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SUMMARY

A FORTRAN program that can be used to analyze the elastic scattering of spin zero particles from an atomic nucleus is presented. The nucleus is represented by the nuclear optical model in the form of a Saxon-Woods volume potential plus a surface interaction potential whose radial dependence is in the form of the derivative of a Saxon-Woods form factor. There are available four independent parameters of each of the two potentials; V and W, the strengths of the real and imaginary parts of the potential, R, the radius of the potential, and a, the diffuseness parameter. Provision is made for varying these parameters over a chosen grid in the parameter space or for searching for a best fit to experimental cross section data by minimizing the chi-squared deviation as a function of chosen parameters. Since most of the computation time is expended in integrating the radial wave equation, the method of integration chosen is about twice as fast as the commonly used Runge-Kutta method.

INTRODUCTION

This report describes a FORTRAN program, ELSA, developed at the Lewis Research Center for the analysis of elastic scattering of spin zero particles against atomic nuclei, which are represented by the nuclear optical model. ELSA was developed to analyze experimental scattering cross section data in terms of the optical-model parameters, and, for this purpose, includes a search procedure for obtaining good fits to experimental data. The calculations are repeated many times in the search procedure, so the program was designed to use a method of integration (ref. 1) that is about twice as fast as the commonly used Runge-Kutta method (ref. 2). Since most of the computation time is expended in the integration of the radial wave equation, this method leads to a relatively fast program.

The program calculates the differential elastic cross section $\sigma_{th}(\theta)$ as a function of the center of mass scattering angle θ for spin zero particles with arbitrary mass, charge, and nonrelativistic energy scattered from a nucleus at rest with arbitrary mass and charge. The incident and target particles are taken

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to have an interaction in the form of a two-body potential, which is taken to be a complex nuclear potential containing a volume term of the Saxon-Woods (ref. 3) type, and a surface term whose radial dependence is in the form of the derivative of the Saxon-Woods form factor. The spin of the target nucleus is neglected in accordance with the usual formulation of the nuclear optical model. If the incident particle is charged, the interaction includes a coulomb potential between an incident point charge and a target sphere of constant charge density.

The potential parameters available are V and W, the real and imaginary constants that fix the depth of the potential well; R, the radius of the potential well; and a, the constant that controls the diffuseness of the surface of the well. Each of these parameters can be specified independently for the volume and surface potentials. The parameters may be varied by fixed amounts by means of a grid variation to cover a specified set of points in the eight-dimensional parameter space. It is also possible to search the parameter space for a set of parameters that minimizes χ^2 (chi-squared deviation) computed from the experimental differential scattering cross section, $\sigma_{ex}(\theta)$, and the calculated $\sigma_{th}(\theta)$.

MATHEMATICAL FORMULATION

General Scattering Formulas

First, the basic equations of scattering for charged, spin zero particles will be reviewed. The interaction between the particles is taken to be of the form

$$V = V_N(r) + V_c(r) \tag{1}$$

where V_N is the complex nuclear potential and V_c is the coulomb potential, both depending only on the distance r between the incident particle and the target particle. The Schrödinger equation for this case is

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\Psi = E\Psi \tag{2}$$

where

$$\mu = \frac{m_p m_T}{m_p + m_T} \tag{3}$$

$$E = \frac{m_T}{m_p + m_T} E_{lab} \tag{4}$$

m_p and m_T are the mass of the incident and target particles, respectively, and E_{lab} is the laboratory energy of the incident particle.

The wave function for the incident particle must be a solution at large val-

ues of r to the Schrödinger equation with $V_N(r) = 0$ and with

$$V_c = \frac{Z_p Z_T e^2}{4\pi\epsilon_o r} \tag{5}$$

where $Z_p e$ is the charge of the incident particle and $Z_T e$ the charge of the target. For convenience, the parameter η is introduced:

$$\eta = \frac{\mu Z_p Z_T e^2}{\hbar^2 k 4\pi\epsilon_o} \tag{6}$$

where k is the wave number in the center of mass system. The incident wave function normalized to one incident particle per unit time per unit area is denoted by Ψ_c; it is also a solution to

$$-\overline{\nabla}^2\Psi_c + \frac{2k\eta}{r}\Psi_c = k^2\Psi_c \tag{7}$$

In this case,

$$\Psi_c = \frac{1}{\sqrt{v}}\Gamma(1 + i\eta)e^{-\eta\pi/2}\, e^{ikz}F[i\eta, 1, ik(r - z)] \tag{8}$$

where v is the velocity of the particle, the z coordinate axis is taken as the direction of the incident particle, and F is the confluent hypergeometric function.

The asymptotic form of Ψ_c can be written as

$$\Psi_c \cong \frac{1}{\sqrt{v}}\left\{e^{i[kz-\eta \ln k(r-z)]}\left[1 - \frac{\eta^2}{ik(r - z)}\right] + \frac{f_c(\theta)}{r}\, e^{i(kr-\eta \ln 2kr)}\right\} \tag{9}$$

The Rutherford scattering amplitude here is denoted by $f_c(\theta)$ and is

$$f_c(\theta) = \frac{-\eta}{2k \sin^2\frac{\theta}{2}}\, e^{-i\eta \ln[\sin^2(\theta/2)]}\, e^{2i\sigma_o} \tag{10}$$

The zero angular momentum coulomb phase shift σ_o is obtained by setting the orbital angular momentum quantum number L equal to zero in the usual coulomb phase shift formula:

$$\sigma_L = \arg \Gamma(L + 1 + i\eta) \tag{11}$$

The partial wave expansion of Ψ_c is

$$\Psi_c = \frac{1}{\sqrt{v}} \sum_{L=0}^{\infty} (2L + 1) i^L e^{i\sigma_L} F_L(\eta, kr) \frac{P_L(\cos\,\theta)}{kr} \tag{12}$$

where σ_L is the coulomb phase shift, $F_L(\eta, kr)$ is the regular coulomb function, and $P_L(\cos\,\theta)$ are the Legendre polynomials.

The total wave function Ψ_{tot} can be written as the sum of the incident wave and a scattered wave, where the scattered wave includes only deviations from pure Rutherford scattering and interference terms. This can be written in the partial wave expansion:

$$\Psi_{tot} = \Psi_c + \Psi_{scatt} = \frac{1}{\sqrt{v}} \sum_{L=0}^{\infty} (2L + 1) i^L e^{i\sigma_L} \Psi_L(r) \frac{P_L(\cos\,\theta)}{kr} \tag{13}$$

The radial wave function Ψ_L must satisfy the condition that only the outgoing wave is modified by the nuclear interaction, which means that the asymptotic expression is

$$\Psi_L \cong F_L(\eta, kr) + \frac{B_L}{2i}\left[G_L(\eta, kr) + iF_L(\eta, kr)\right] \tag{14}$$

where B_L is a complex constant and G_L is the irregular coulomb function.

When the asymptotic forms for the regular and irregular coulomb functions are introduced,

$$F_L \cong \sin\left(kr - \eta\,\ln\,2kr - \frac{L\pi}{2} + \sigma_L\right) \tag{15}$$

$$G_L \cong \cos\left(kr - \eta\,\ln\,2kr - \frac{L\pi}{2} + \sigma_L\right) \tag{16}$$

the radial wave function becomes

$$\Psi_L \cong \sin\left(kr - \eta\,\ln\,2kr - \frac{L\pi}{2} + \sigma_L\right) + \frac{B_L}{2i}\, e^{i\left[kr - \eta\,\ln\,2kr - (L\pi/2) + \sigma_L\right]} \tag{17}$$

It is possible to express Ψ_L in another manner in the asymptotic region, namely, as a regular coulomb wave whose phase has been shifted by an amount given by the nuclear phase shift δ_L. This expression is

$$\Psi_L \cong A_L\,\sin\left(kr - \eta\,\ln\,2kr - \frac{L\pi}{2} + \sigma_L + \delta_L\right) \tag{18}$$

where A_L is a complex constant and δ_L the complex nuclear phase shift. A comparison of the coefficients of the incoming and outgoing waves in equations (17) and (18) yields

$$\left.\begin{aligned} B_L &= e^{2i\delta_L} - 1 \\ A_L &= e^{i\delta_L} \end{aligned}\right\} \tag{19}$$

Thus Ψ_L in the asymptotic region can be expressed as

$$\Psi_L \cong \sin\left(kr - \eta \ln 2kr - \frac{L\pi}{2} + \sigma_L\right) + \sin \delta_L e^{i\left[kr-\eta \ln 2kr-(L\pi/2)+\sigma_L+\delta_L\right]} \tag{20}$$

The asymptotic form of the wave function can be written in terms of the asymptotic form of the incident wave and the coefficient B_L as follows:

$$\Psi_{tot} \cong \frac{1}{\sqrt{v}} \left\{e^{i[kr-\eta \ln k(r-z)]}\left[1 - \frac{\eta^2}{ik(r - z)}\right]\right\}$$
$$+ \frac{1}{\sqrt{v}} \frac{e^{i(kr-\eta \ln 2kr)}}{r}\left[f_c(\theta) + \sum_{L=0}^{\infty} (2L + 1)e^{2i\sigma_L} \frac{B_L}{2ik} P_L(\cos \theta)\right] \tag{21}$$

The scattered wave is the portion containing the e^{ikr}/r term, and the differential cross section is given by

$$\sigma_{th}(\theta) = |f_c(\theta) + f_N(\theta)|^2 \tag{22}$$

where

$$f_N(\theta) = \frac{1}{k}\sum_{L=0}^{\infty} (2L + 1)e^{2i\sigma_L} \frac{B_L}{2i} P_L(\cos \theta) \tag{23}$$

and $f_c(\theta)$ is given by equation (10).

The pure coulomb cross section is

$$\sigma_c(\theta) = |f_c(\theta)|^2 \tag{24}$$

Nuclear and Coulomb Potentials

The nuclear potential is taken to be

$$V_N(r) = -\left(\frac{V_1 + iW_1}{1 + \exp\left[\frac{r - R_1}{a_1}\right]} + \frac{(V_2 + iW_2)4\exp\left[\frac{r - R_2}{a_2}\right]}{\left\{1 + \exp\left[\frac{r - R_2}{a_2}\right]\right\}^2}\right) \tag{25}$$

The numbers V_1, V_2 and W_1, W_2 are positive for an attractive potential.

The coulomb potential is taken to be that of a sphere of radius R_c having a uniform charge density:

$$V_c = \frac{Z_p Z_T e^2}{4\pi\epsilon_o R_c}\frac{1}{2}\left(3 - \frac{r^2}{R_c^2}\right) \qquad r < R_c$$

$$= \frac{Z_p Z_T e^2}{4\pi\epsilon_o r} \qquad r > R_c \tag{26}$$

PROGRAM DESCRIPTION

General Description

The program is written in FORTRAN II language and, as listed in appendix A, is arranged to operate with the Lewis Research Center 7090 monitor system. The function of the monitor is to coordinate compiler and assembler processing and to provide a means for initiating execution of object programs. The monitor system also provide an error package whose function is to detect and control certain types of errors in FORTRAN programs. The error control cards used with ELSA are designated *MAJOR UNDER (NO PRINT) and *ZERO DIVIDE. These correct a floating-point major underflow and a division by zero by setting the result to zero. The library tape functions used are the standard FORTRAN II functions, with the exception of a subroutine called PLOTMY (X,Y,K,P). This subroutine is part of the library tape of the Lewis Monitor System (ref. 4) and is available for general use. Where this subroutine is not on the library tape, the program can be run by changing statement 715 (card 7-073) to read "RETURN," deleting cards 7-074 and 7-075 in subroutine SEVEN, and deleting subroutine PLOT7. The last input data card, with the data for the horizontal and vertical scales of the plot, will not be used if this change is made.

ELSA consists of a main routine and 10 subroutines. The main routine calls the subroutines in the proper sequence and also provides for a sequential variation of the parameters V_i, W_i, R_i, and a_i $(i = 1,2)$. The subroutines and the calculations each performs are listed as follows:

Subroutine ONE	Reads in data cards, performs a reduction of input data
Subroutine TWO	Computes coulomb phase shifts and coulomb wave functions
Subroutine THREE	Tabulates coulomb potential and r^2
Subroutine FOUR	Tabulates optical potential form factors, obtains power-series coefficients
Subroutine FIVE	Tabulates effective kinetic energy
Subroutine SIX	Computes radial wave function by integrating Schrödinger equation, then computes scattering amplitudes
Subroutine SEVEN	Computes cross section χ^2, calls PLOT7
Subroutine PLOT7	Sets up PLOTMY
Subroutine PLOTMY	Furnishes a plot of σ_{ex} against θ_{ex}, and σ_{th} against θ_{th}
Subroutine EIGHT	Provides a search on any combination of the parameters V_i, W_i, R_i, and a_i $(i = 1,2)$ by minimizing χ^2

Details of Specific Subroutines

Subroutine ONE. - This routine reads in the data cards and performs a reduction of the input data to the forms used by the program. It determines the size of the increment Δr ($\equiv \delta$, FORTRAN name ADD) used in the integration. This is done by setting $\delta = \delta_0/k$ and rounding the result to three figures. The dimensionless input parameter $\delta_0 \equiv$ DEL is approximately the size of the integration increment in terms of the dimensionless variable kr. The subroutine also computes normalization factors for the radial wave functions. The input data used are listed in the section INPUT DATA.

Subroutine TWO. - The coulomb phase shifts are computed by using Stirling's formula to obtain a value for σ_{50} from equation (11) and then by using the recurrence relation

$$\sigma_{L-1} = \sigma_L - \tan^{-1}\frac{\eta}{L} \equiv \mathrm{AS(L)} \tag{27}$$

to obtain the values for the lower values of L. The designation listed to the right of the ($\equiv$) sign is the FORTRAN name of the variable.

The regular and irregular coulomb wave functions (F_L,G_L) are computed at two values of r, namely, r_{max} and $r_{max} - 2\delta$ (ARM and ARM -2 ADD). In order to furnish starting values for the use of the recurrence relation, the values of the coulomb wave functions for $L = 0$ and $L = 1$ (F_0,F_1,G_0,G_1) are computed at these

points by using the asymptotic relations (ref. 5)

$$\left.\begin{aligned} F_L &= V_L \cos \Theta_L + U_L \sin \Theta_L \equiv FF(N,L+1) \\ G_L &= U_L \cos \Theta_L - V_L \sin \Theta_L \equiv GG(N,L+1) \end{aligned}\right\} \tag{28}$$

where N is equal to 1 or 2 depending on the radial position, and

$$\Theta_L = kr - \eta \ln 2kr - \frac{\pi L}{2} + \sigma_L \tag{29}$$

The variables U_L and V_L used to calculate the coulomb wave functions are given by the series

$$U_L + iV_L = (1 + C_{1,L} + C_{1,L}C_{2,L} + C_{1,L}C_{2,L}C_{3,L} + \cdots \tag{30}$$

$$C_{J,L} = \frac{(i\eta - L + J - 1)(i\eta + L + J)}{i2krJ} \tag{31}$$

The maximum number of terms in the asymptotic series is set by the input control NN1. The series is terminated when the magnitude of any term exceeds that of the previous term, or when the ratio of the magnitude of any term to the magnitude of the sum of the series becomes less than the input number BB5. If neither of these terminations occurs and the number of terms actually reaches NN1, the value of ARM is increased to ARM + 6 × NN2 × ADD, and a new series is computed. The values of F_0, F_1, G_0, and G_1 are checked by computing the Wronskian, and if they are not sufficiently accurate, the value of ARM is increased to ARM + 6 × NN2 × ADD, and the coulomb functions are computed at this new point. The values of F_L and G_L are then obtained from the recurrence relation

$$L\sqrt{(L+1)^2 + \eta^2}\, U_{L+1} = (2L+1)\left[\eta + \frac{L(L+1)}{kr}\right]U_L - (L+1)\sqrt{L^2 + \eta^2}\, U_{L-1} \tag{32}$$

where

$$U_L = F_L \quad \text{or} \quad G_L$$

The recurrence relations can be used to obtain accurate values of G_L by recurring upward from G_0 and G_1. Since the F_L cannot be computed accurately by recurring upward, arbitrary starting values are assigned to F_{LRM+10} and F_{LRM+11}, where LRM is the maximum value of L to be used in the program and is determined from input parameters. The recurrence relations are used to generate the F_L downward, which are then normalized to the value of F_0 computed by the asymptotic series. Each F_L is then checked to see if the Wronskian satisfies the following criterion:

$$\left| F_{L-1}G_L - F_LG_{L-1} - \left(1 + \frac{\eta^2}{L^2}\right)^{-1/2} \right| < 10^{-5} \tag{33}$$

If any of the F_L fail this test, the starting value of L for the downward recurrence on F_L is increased by 10, and the process is repeated. If the starting value of L for the downward recurrence becomes greater than $L = 100$, the program value of ARM is increased and the following statement written out: RECURRENCE RELATIONS FOR COULOMB WAVE FUNCTIONS HAVE FAILED, INCREASE RMAX. If the value of ARM is ever increased to the point where the number of storage locations allocated to V_c and r^2 in subroutine THREE will be exceeded, the program proceeds to the next set of data, and the following statement is written out: ARM EXCEEDS AVAILABLE STORAGE FOR POTENTIALS, PROCEED TO NEXT CASE.

Subroutine THREE. - The values of the coulomb potential V_c and of r^2 are tabulated at all mesh points. The coulomb potential is added to the constant kinetic energy term and stored in the forms

$$\frac{\delta^2}{12}\left(k^2 - \frac{3k\eta}{R_c} + \frac{k\eta r^2}{R_c^3}\right) \equiv VC(I) \qquad r < R_c$$

$$\frac{\delta^2}{12}\left(k^2 - \frac{2k\eta}{r}\right) \equiv VC(I) \qquad r > R_c \tag{34}$$

Subroutine FOUR. - The Saxon-Woods form factor

$$f_1(r) = \frac{1}{1 + \exp\left[\frac{r - R_1}{a_1}\right]} \equiv SS(I) \tag{35a}$$

is tabulated at each mesh point. The surface interaction form factor,

$$f_2(r) = \frac{4 \exp\left[\frac{r - R_2}{a_2}\right]}{\left\{1 + \exp\left[\frac{r - R_2}{a_2}\right]\right\}^2} \equiv TT(I) \tag{35b}$$

is also tabulated at each mesh point where it is significant.

To start the integration of the radial wave function in subroutine SIX, a power-series solution is used to get initial values of the wave function. This solution uses a power-series expansion for the nuclear potential at a starting point that must be inside the nuclear potential well, since the series converges only for $r < R_1$. Since the starting value of r is usually small, the surface potential is neglected in obtaining the initial value of the wave function. The coefficients for the power-series expansion of the Saxon-Woods form factor are computed by using

$$\frac{1}{1 + \exp\left[\frac{r - R_1}{a_1}\right]} = \sum_{m=0}^{\infty} \gamma_m r^m \tag{36}$$

The coefficients γ_m can be expressed in terms of the form factor evaluated at $r = 0$. The exponential evaluated at $r = 0$ is denoted by

$$\exp\left[- \frac{R_1}{a_1}\right] = E \tag{37}$$

The γ_m are then given by

$$\gamma_m \equiv \gamma_M = \frac{1}{M!\,(a_1)^M} \left(\frac{1}{1+E}\right) \sum_{J=1}^{\infty} A_J^M \, J!\left(\frac{-E}{1 + E}\right)^J \equiv CC(1,M + 1) \tag{38}$$

The coefficients A_J^M satisfy the recurrence relations

$$A_J^M = JA_J^{M-1} + A_{J-1}^{M-1} \equiv AC(J) \tag{39}$$

with

$$A_M^M = 1 = A_1^M$$

and

$$\begin{aligned} A_J^M &= 0 \qquad J > M \\ &= 0 \qquad J < 1 \end{aligned}$$

Subroutine FIVE. - The nuclear potential contribution to the effective kinetic energy term in the Schrödinger equation is obtained and added to the coulomb potential. This is stored in the following forms:

$$VC(I) + \frac{2\mu}{\hbar^2} \frac{\delta^2}{12} \left[V_1 f_1(r) + V_2 f_2(r)\right] \equiv VV(I) \tag{40a}$$

$$\frac{2\mu}{\hbar^2} \frac{\delta^2}{12} \left[W_1 f_1(r) + W_2 f_2(r)\right] \equiv WW(I) \tag{40b}$$

where VC(I) is computed in subroutine THREE, and $f_1(r)$ and $f_2(r)$ are computed in subroutine FOUR. The power-series coefficients for the nuclear form factor are combined with the strength of the potential and stored as

$$\frac{2\mu}{\hbar^2} V_1 \gamma_M \equiv DD(1,M + 1) \tag{41a}$$

$$\frac{2\mu}{\hbar^2} W_1 \gamma_M \equiv DD(2,M + 1) \tag{41b}$$

Subroutine SIX. - The radial wave functions are computed for each value of L from zero to L_{max} by integrating the Schrödinger equation, starting near the origin and proceeding out to a point well beyond the range of the nuclear potential. The starting values for the wave function are obtained from a power-series solution to the radial wave equation at the starting value of r. The differential equation for the radial wave function χ_L is

$$\left[\frac{d^2}{dr^2} + k^2 - k^2 \frac{V(r)}{E} - \frac{L(L + 1)}{r^2}\right]\chi_L = 0 \tag{42}$$

where

$$\chi_L = C_L \Phi r^{L+1} = C_L \sum_{n=0}^{\infty} \Phi_n r^{n+L+1} \tag{43}$$

in which C_L is the normalization constant given in equation (48). The effective kinetic energy terms are expanded in powers of r as follows:

$$k^2 - k^2 \frac{V(r)}{E} = k^2 - \frac{3k\eta}{R_c} + \frac{k\eta r^2}{R_c^3} - \frac{k^2}{E}(V_1 + iW_1)\sum_{m=0}^{\infty} \gamma_m r^m \qquad r < R_c \tag{44}$$

The following recurrence relations are found for the Φ_n:

$$\Phi_n^+ = \frac{1}{n(n + 2L + 1)}\left[-k^2\Phi_{n-2}^+ + \frac{3k\eta}{R_c}\Phi_{n-2}^+ - \frac{k\eta}{R_c^3}\Phi_{n-4}^+ - \sum_{m=0}^{n-2}\left(v_m^+\Phi_{n-2-m}^+ - v_m^-\Phi_{n-2-m}^-\right)\right] \tag{45a}$$

$$\Phi_n^- = \frac{1}{n(n + 2L + 1)}\left[-k^3\Phi_{n-2}^- + \frac{3k\eta}{R_c}\Phi_{n-2}^- - \frac{k\eta}{R_c^3}\Phi_{n-4}^- - \sum_{m=0}^{n-2}\left(v_m^+\Phi_{n-2-m}^- + v_m^-\Phi_{n-2-m}^+\right)\right] \tag{45b}$$

The quantities in equations (45) appear in the program as

$$\Phi_n = \Phi_n^+ + i\Phi_n^- \equiv BB(1,N + 1) + iBB(2,N + 1) \tag{46}$$

and

$$\nu_m^+ + i\nu_m^- = + \frac{k^2}{E} V_1\gamma_m + \frac{ik^2}{E} W_1\gamma_m \equiv DD(1, M + 1) + iDD(2, M + 1) \tag{47}$$

The values for Φ_0 are taken to be

$$\Phi_0^+ = 1.0 \qquad \Phi_0^- = 0$$

The starting values for the wave function are normalized to the coulomb function normalization so that

$$\chi_L = \sqrt{\frac{2\pi\eta}{e^{2\pi\eta} - 1}} \frac{\sqrt{1^2 + \eta^2}}{1(2 \cdot 1 + 1)} \cdot \cdot \cdot \frac{\sqrt{L^2 + \eta^2}}{L(2 \cdot L + 1)} (kr)^{L+1}\Phi = C_L(kr)^{L+1}\Phi \tag{48}$$

The integration method is that of successive extrapolation; that is, the value of χ_L at any given point is extrapolated from the values at two previous points and the difference in r. The relations are obtained from Taylor series expansions of $\chi_L(r \pm \delta)$ about the point r and from use of the differential equation to evaluate the second derivative appearing in the expansion (ref. 1). The complex function χ_L is denoted as

$$\chi_L \doteq \chi_L^+ + i\chi_L^- \tag{49}$$

The equation to be solved can be written with the subscript L temporarily suppressed in the form

$$\left[\frac{d^2}{dr^2} + \eta^+(r) + i\eta^-(r)\right](\chi^+ + i\chi^-) = 0 \tag{50}$$

If

$$q(r) \equiv 1 + \frac{\delta^2}{12} \eta^+(r) \tag{51a}$$

$$p(r) \equiv \frac{\delta^2}{12} \eta^-(r) \tag{51b}$$

the solutions are

$$\chi^{\pm}(r + \delta) = \frac{X^{\pm}(r)q(r + \delta) \pm X^{\mp}(r)p(r + \delta)}{q^2(r + \delta) + p^2(r + \delta)} \tag{52}$$

where

$$X^{\pm}(r) = [12 - 10q(r)]X^{\pm}(r) - q(r - \delta)X^{\pm}(r - \delta) \pm 10p(r)X^{\mp}(r) \pm p(r - \delta)X^{\mp}(r - \delta) \tag{53}$$

By comparing equation (50) to the previous form of the radial equation (eq. (42)), it is seen that

$$\eta^{+}(r) = k^2 + \frac{k^2}{E}\left[\mathrm{Re}\ V_N(r) - V_c(r)\right] - \frac{L(L + 1)}{r^2} \tag{54a}$$

$$\eta^{-}(r) = + \frac{k^2}{E}\ \mathrm{Im}\ V_N(r) \tag{54b}$$

The integration is carried out to the place where $r = r_{max}$, and the values of the wave function at the last two mesh points are stored.

The value of the scattering amplitude B_L is obtained by evaluating equation (14) at each of the last two mesh points. When equation (14) is written explicitly with an arbitrary normalizing factor $\overline{C}_L$, the equation becomes

$$\overline{C}_L\left(X_L^{+} + iX_L^{-}\right) = F_L + \left(\frac{B_L^{+} + iB_L^{-}}{2i}\right)(G_L + iF_L) \tag{55}$$

Using this relation at two values of r enables elimination of C_L and solution for B_L. For a specified value of L, this solution is

$$B^{+} + iB^{-} = \frac{2i\left[\left(X_1^{+} + iX_1^{-}\right)F_2 - \left(X_2^{+} + iX_2^{-}\right)F_1\right]}{\left(X_2^{+} + iX_2^{-}\right)(G_1 + iF_1) - \left(X_1^{+} + iX_1^{-}\right)(G_2 + iF_2)} \equiv BP + iBM \tag{56}$$

where the subscripts refer to the last mesh point (2) and the previous mesh point (1).

Subroutine SEVEN. - This subroutine computes the differential elastic cross sections as given by equations (22) and (23) for each of the experimental angles. A value of χ^2 is computed as follows:

$$\chi^2 = \sum_{\theta=\theta_{ex,i}}^{\theta_{ex,N}} W(\theta_{ex,i})\left[\frac{\sigma_{th}(\theta_{ex,i}) - \sigma_{ex}(\theta_{ex,i})}{\sigma_{ex}(\theta_{ex,i})}\right]^2 \tag{57}$$

where $W(\theta_{ex,i})$ is an assigned weight factor, σ_{th} is the calculated cross section, and σ_{ex} is the experimental cross section at each experimental angle θ_{ex}.

If a search over the optical model parameters is desired, subroutine EIGHT is entered. At the end of the search, or if no search is used, the differential

elastic cross section is computed at θ_{th}, where θ_{th} is a calculated set of evenly spaced angles if KDCAL $\neq 0$, and otherwise θ_{th} is equal to θ_{ex} if KDCAL = 0. The pure coulomb differential cross section, as given by equation (24), is computed at each angle θ_{th}, and the angles, elastic cross sections, coulomb cross sections, and ratio of elastic to coulomb cross sections are printed out.

Subroutine EIGHT. - The search routine provides a variation of any of the parameters V_i, W_i, a_i, and R_i $(i = 1,2)$, which are denoted by α_j in the following discussion. First α_1 is changed to $\alpha_1 + d\alpha_1$, where $d\alpha_1$ is input data. The subroutine returns to the optical model program, and a new set of $\sigma_2(\theta)$ and a value of χ_2^2 are calculated. The value of χ_2^2 is compared with χ_1^2, and if it is smaller, the variable α_1 is changed to $\alpha_1 + 2d\alpha_1$ and the process repeated. (If $\chi_2^2 > \chi_1^2$, the variation is made in the opposite direction, that is, α_1 is changed to $\alpha_1 - d\alpha_1$.) The variations are continued in the same direction until the value of the current χ^2 is larger than the previous χ^2.

The value of α_1 for which χ^2 is a minimum is then interpolated by fitting a parabola to the last three values of $\chi^2(\alpha_1)$.

With the value of α_1 fixed at the interpolated value of α_1 (and keeping the six other α_j fixed at the initial values), the value of α_2 is changed to $\alpha_2 + d\alpha_2$. Values of σ_{th} and χ^2 are computed, and the same process as described for α_1 is carried out. The procedure is repeated for each of the desired α_j. At the end of one of these circuits, the process can be repeated if desired with the same $d\alpha_j$ or with each $d\alpha_j$ reduced by a constant factor. The search can be repeated as many times as desired and can be terminated by limiting the number of circuits, or when χ^2 fails to be reduced by some predetermined input factor. When the search is terminated, the program returns to subroutine SEVEN, which prints out (and plots) the final cross section.

Subroutine PLOTMY (X,Y,K,P) (ref. 4). - This routine is a general plotting subroutine that is part of the Library Tape of the Lewis Monitor System. Its use here is to furnish plots of $\log_{10} \sigma_{ex}$ against θ_{ex} and $\log_{10} \sigma_{th}$ against θ_{th}. In the PLOTMY subroutine, the variable X is plotted down the page, and Y is plotted across the page; K is an array controlling the possible options of PLOTMY, and P is an array controlling the vertical and horizontal scales.

The subroutine PLOTMY is called by subroutine PLOT7, which prepares the cross-section data in a form suitable for PLOTMY.

Subroutine PLOT7. - This subroutine arranges to put the values of $-\log_{10} \sigma_{ex}(\theta)$ and $-\log_{10} \sigma_{th}(\theta)$ into the array X(I) and the values of θ_{ex} and θ_{th} into the array Y(I). The proper values of K(I) are set to plot two curves with the X and Y scales specified by input controls P(I). The input con-

trols P(I) are read in by subroutine PLOT7. If the subroutine PLOTMY is not available to the program, subroutine PLOT7 should be removed along with cards 7-074 and 7-075. Card 7-073 should be changed to read 715 RETURN. The input data card with the plot controls, P(I), will not be used if this change is made.

The input controls must be integers. A convenient method of selecting the control numbers is first to choose the desired increment $\Delta\theta$ in the horizontal scale that will be equal to one printing position (there are 100 printing positions horizontally on the page). P(11) must be chosen to be an integer that is $\Delta\theta$ times a power of 10. P(9) is then the value such that 6 - P(9) gives the correct exponent of 10 in the equation

$$P(11) = \Delta\theta \times 10^{6-P(9)}$$

The value of P(10) is then obtained from the desired starting value (N) of θ by the equation

$$P(10) = N \times 10^{6-P(9)}$$

These values set up the horizontal scale. The values for P(8), P(6), and P(7) controlling the vertical scale are set up in a similar manner. There are 60 line spaces per page on the vertical scale. But in contrast to the horizontal scale, which is limited to 100 points, the vertical scale has no such limitation and can be made to cover several pages continuously.

INPUT DATA

Description

Units for the input data are as follows:

Energy	Mev
Potential strength	Mev
Mass	amu
Length	fermis
Charge	dimensionless multiples of electron charge
Angle	degrees
Cross sections	millibarns

The data are input from tape 7, which is prepared from IBM cards as follows:

Card 1	FORMAT (13A6) title card - 78 Hollerith characters to identify the run
Card 2	FORMAT (15I5) control numbers (the subroutines in which these are used are in parenthesis)
NN1	maximum number of terms in asymptotic series for coulomb wave functions (2)
NN2	number of triplets of mesh points to increase r_{max} if asymptotic series does not converge (2)
NN3	0, no surface interaction; 1, yes surface interaction (4)
NN4	maximum number of terms in form-factor power series (4)
NN5	0, no search; 1, yes search using subroutine EIGHT (7,8)
NN6	number of search circuits before search interval is reduced (8)
NN7	maximum number of circuits in search (8)
NN8	maximum number of terms in wave-function power series (6)
NT1	number of angles for final calculated angular distribution (7)
NTT	number of experimental angles (7)
INKODE	0, do not read in experimental data; 1, read in experimental data (1)
KDPPLT	0, no plot is given; 1, yes plot
KDGRD	0, no rough grid; 1, yes rough grid
KDCAL	0, $\theta_{th} = \theta_{ex}$; 1, $\theta_{th} \neq \theta_{ex}$
Card 3	FORMAT (15I5) control number (this card can be blank if no grid variation is used)
NV1X	number of grid points for V_1 (MAIN)
NW1X	number of grid points for W_1 (MAIN)
NR1X	number of grid points for R_1 (MAIN)
NA1X	number of grid points for a_1 (MAIN)
NV2X	number of grid points for V_2 (MAIN)
NW2X	number of grid points for W_2 (MAIN)

NR2X number of grid points for R_2 (MAIN)

NA2X number of grid points for a_2 (MAIN)

Card 4 FORMAT (8F10.0) basic data

AV1 $|V_1|$, real strength of Saxon well (5)

AW1 $|W_1|$, imaginary strength of Saxon well (5)

AR1 R_1, radius of Saxon well (4)

AA1 a_1, diffuseness of Saxon well (4)

DV1 grid or search increment of V_1 (8 or MAIN)

DW1 grid or search increment of W_1 (8 or MAIN)

DR1 grid or search increment of R_1 (8 or MAIN)

DA1 grid or search increment of a_1 (8 or MAIN)

Card 5 FORMAT (8F10.0) basic data

AV2 $|V_2|$, real strength of surface well (5)

AW2 $|W_2|$, imaginary strength of surface well (5)

AR2 R_2, radius of surface well (4)

AA2 a_2, diffuseness of surface well (4)

DV2 grid or search increment of V_2 (8 or MAIN)

DW2 grid or search increment of W_2 (8 or MAIN)

DR2 grid or search increment of R_2 (8 or MAIN)

DA2 grid or search increment of a_2 (8 or MAIN)

Card 6 FORMAT (8F10.0) basic data

AEE laboratory energy of incident particle (1)

ARC radius of charge distribution (3)

DEL desired mesh size δ_o as a fraction of kr (1)

ARR radius at which mesh size is doubled (6)

AMP mass of incident particle (1)

AZP charge of incident particle (1)

AMT mass of target particle (1)

AZT charge of target particle (1)

Card 7 FORMAT (8F10.0) basic data

AT1 initial angle for calculated angular distribution (7)

DT1 increment in angle for final angular distribution (7)

Card 8 FORMAT (8E10.0) convergence parameters

BB1) determine $r_{max} \geq R_1 + a_1B_1 + B_2$ (1)

BB2) determine $r_{max} \geq R_2 + a_2B_1 + B_2$ (1)

BB3 determine $r_{max} \geq B_3 + (\eta/k)$ (1)

BB4 determine $LRM = kr_{max} + B_4$ (1)

BB5 convergence parameter for asymptotic series for coulomb wave functions (2)

BB6 form-factor cutoff (4)

BB7 convergence parameter for wave-function power series (6)

BB8 convergence parameter for scattering amplitudes (6)

Card 9 FORMAT (8E10.0) convergence parameters

BB9 reduction factor for search interval (8)

B10 convergence factor on decrease in χ^2 by search program (8)

B11 determine starting radius for integration from $r = B_{11}L(\delta_o/k)$; note B11 should always be greater than 0.4 (6)

If INKODE = 0, there are no cards with experimental data to be read in. If INKODE $\neq$ 0, cards containing experimental data will be required. The number of these cards is as follows:

NTT even, there are NTT/2 cards

NTT odd, there are (NTT + 1)/2 cards

Each card contains two angles, two cross sections, and two weight factors.

Cards 10, etc.	FORMAT (6F10.0)
HH(1)	first experimental angle (7)
XX(1)	first experimental cross section (7)
WX(1)	first weight factor (7)
HH(2)	second experimental angle (7)
XX(2)	second experimental cross section (7)
WX(2)	second weight factor (7)

If KDPLOT $\neq 0$, there is one more card:

Card PLOT	FORMAT (6F10.0) controls for PLOT7 subroutine
P(6)	determines vertical scale factor, $10^{6-P(6)}$
P(7)	determines vertical scale starting value; let M be the first integer greater than $\log_{10} \sigma_{max}$; then P(7) is the negative number such that $\lvert P(7) \rvert = M \times 10^{6-P(6)}$
P(8)	determines desired increment $\Delta(\log_{10} \sigma)$ in vertical scale equal to one line space, $P(8) = \Delta(\log_{10} \sigma)10^{6-P(6)}$
P(9)	determines horizontal scale factor, $10^{6-P(9)}$
P(10)	determines horizontal scale starting value; let N be desired starting value for θ, then $P(10) = N \times 10^{6-P(9)}$
P(11)	determines desired increment $\Delta\theta$ in horizontal scale equal to one printing position, $P(11) = \Delta\theta \times 10^{6-P(9)}$

Sample

A sample data set of input data is listed in appendix B. There are nine cards corresponding to cards 1 to 9 as described in the previous section, 18 cards containing the experimental angles, cross sections, and weight factors, and a final card with the PLOT controls. The values of the various controls numbers and convergence parameters, which appear on cards 2, 8, and 9, are typical values that have been found satisfactory and that can be used as guides in choosing these parameters.

SAMPLE OUTPUT DATA

A sample set of output data from the program is listed following the sample input data listing (appendix B). Not all the possible output described appears in the sample case.

The title card is printed at the beginning of each case. Following this on the first page is a labeled print-out of the input data contained on cards 1 to 9. (Card 3 is printed here only if a parameter grid is being used.) The experimental angles, cross sections, and weight factors are printed on the second page.

At the top of the third page some of the output from subroutine ONE appears. Here are printed values of the wave number $k \equiv$ AKK; the mesh size, $\Delta r \equiv$ ADD; the coulomb parameter, $\eta \equiv$ AZZ; the normalization factor for the $L = 0$ radial wave function, ACC; the radius at which the mesh size is doubled, ARR; the matching or maximum radius, ARM; the value of the index of the doubling radius, IRR; the value of the index of the maximum radius, IRM; and the maximum L value to be used, LRM.

The next output comes from subroutine TWO. If the recurrence relations give values of F_L and G_L whose Wronskian is greater than 10^{-5}, there is an output statement noting this and noting that ARM has been increased. If the value of ARM is increased beyond the storage assigned to the potentials, there will be an output statement noting this fact, and the program will proceed to the next set of data (if any). Since it is possible for ARM to be increased with no output statement, there is always a write-out of the final values of ARM and IRM at the completion of subroutine TWO.

The final values of the coulomb radius ARC and the index IRC are written out from subroutine THREE after ARC has been adjusted to be at one of the mesh points.

Next there is output from subroutine SIX. Each time the power series used to obtain a starting value for the radial wave function fails to converge, the starting value for r is decreased and a new power series is computed. The total number of times this happens (for all L values) is printed out as MMM. If the value of r is ever decreased to a value too small for the mesh size used, the computation stops, the statement POWER SERIES FAILED TO CONVERGE IN SIX is printed out, and the current values of MMM and L are printed out. There is a provision for cutting off the number of partial waves used by the program whenever the scattering amplitude becomes sufficiently small. Therefore, the maximum value of L that can be used is printed out as LRM, and the number of partial waves actually used is printed out as LMAX.

If a search or a grid is being used, the values of the parameters and the value of $\chi^2 \equiv$ ERROR are printed at each point of the parameter space. When the search program is being used, the interpolated values of the χ^2 and the parameter being varied are printed whenever an interpolation is made.

When a calculation with a single parameter set or with a search procedure is completed, the calculated values of the elastic cross section, the coulomb cross section, and the ratio of elastic to coulomb cross section, along with the corresponding center of mass angles, are printed out. A plot of the cross sections

against angle is printed if desired. No print-out or plot of the cross section appears if a parameter grid is used.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, October 9, 1963

APPENDIX A

PROGRAM LISTING

```
C     MAIN PROGRAM FOR *ELSA*                                          M-000
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,   C-01
     1        AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                          C-02
     2        BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,    C-03
     3        CC,CN,CS,                                                 C-04
     4        DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,           C-05
     5        ERR,FF,GG,HH,HS,                                          C-06
     6        II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                   C-07
     7        KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,           C-08
     8        LL,LLM,LRM,                                               C-09
     9        NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X   C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                    C-11
     1        QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                       C-12
      DIMENSION BM(51),BP(51),                                          D-01
     1           CC(2,100),CN(90),CS(51),                               D-02
     2           DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),      D-03
     3           QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500), D-04
     4           WW(500),WX(90),                                        D-05
     5           XC(90),XN(90),XX(90)                                   D-06
    1 CALL ONE                                                         M-001
    2 CALL TWO                                                         M-002
      KODE2=KODE2                                                      M-003
      GO TO (1,3),KODE2                                                M-004
    3 CALL THREE                                                       M-005
      IF (KDGRD) 10,4,1                                                M-006
   10 TV1=AV1                                                          M-007
      TW1=AW1                                                          M-008
      TR1=AR1                                                          M-009
      TA1=AA1                                                          M-010
      TV2=AV2                                                          M-011
      TW2=AW2                                                          M-012
      TR2=AR2                                                          M-013
      TA2=AA2                                                          M-014
   12 DO 20  NA2=1,NA2X                                                M-015
      IF (NA2-1) 31,30,31                                              M-016
   30 AA2=TA2                                                          M-017
      GO TO 32                                                         M-018
   31 AA2=AA2+DA2                                                      M-019
   32 DO 20  NR2=1,NR2X                                                M-020
      IF(NR2-1) 34,33,34                                               M-021
   33 AR2=TR2                                                          M-022
      GO TO 35                                                         M-023
   34 AR2=AR2+DR2                                                      M-024
   35 DO 20 NW2=1,NW2X                                                 M-025
      IF (NW2-1) 37,36,37                                              M-026
   36 AW2=TW2                                                          M-027
      GO TO 38                                                         M-028
   37 AW2=AW2+DW2                                                      M-029
   38 DO 20  NV2=1,NV2X                                                M-030
      IF (NV2-1) 40,39,40                                              M-031
   39 AV2=TV2                                                          M-032
      GO TO 41                                                         M-033
   40 AV2=AV2+DV2                                                      M-034
   41 DO 20  NA1=1,NA1X                                                M-035
      IF(NA1-1) 43,42,43                                               M-036
   42 AA1=TA1                                                          M-037
```

```
      GO TO 44
   43 AA1=AA1+DA1
   44 DO 20  NR1=1,NR1X
      IF (NR1-1) 46,45,46
   45 AR1=TR1
      GO TO 47
   46 AR1=AR1+DR1
   47 DO 20  NW1=1,NW1X
      IF (NW1-1) 49,48,49
   48 AW1=TW1
      GO TO 50
   49 AW1=AW1+DW1
   50 DO 20 NV1=1,NV1X
      IF (NV1-1) 52,51,52
   51 AV1=TV1
      GO TO 53
   52 AV1=AV1+DV1
   53 CONTINUE
    4 CALL FOUR
    5 CALL FIVE
    6 CALL SIX
      KODE6=KODE6
      GO TO (1,7),KODE6
    7 CALL SEVEN
      KODE7=KODE7
      GO TO (1,8,20),KODE7
   20 CONTINUE
      GO TO 1
    8 CALL EIGHT
      KODE8=KODE8
      GO TO (4,5), KODE8
      END
```

```
      SUBROUTINE ONE                                                    1-000
C     PROGRAM ONE    DATA REDUCTION                                     1-001
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,    C-01
     1       AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                            C-02
     2       BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,      C-03
     3       CC,CN,CS,                                                   C-04
     4       DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,             C-05
     5       ERR,FF,GG,HH,HS,                                            C-06
     6       II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                     C-07
     7       KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,             C-08
     8       LL,LLM,LRM,                                                 C-09
     9       NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X     C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                     C-11
     1       QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                         C-12
      DIMENSION BM(51),BP(51),                                           D-01
     1          CC(2,100),CN(90),CS(51),                                 D-02
     2          DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),        D-03
     3          QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),   D-04
     4          WW(500),WX(90),                                          D-05
     5          XC(90),XN(90),XX(90)                                     D-06
      DIMENSION TITLE(13)                                                D-07
      READ INPUT TAPE 7,101, (TITLE(I),I=1,13)                          1-002
      WRITE OUTPUT TAPE 6,102, (TITLE(I),I=1,13)                        1-003
      READ INPUT TAPE 7,120, NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,           1-004
     1                       NT1,NTT,INKODE,KDPLT,KDGRD,KDCAL           1-005
      READ INPUT TAPE 7,120, NV1X,NW1X,NR1X,NA1X,NV2X,NW2X,NR2X,NA2X    1-006
      READ INPUT TAPE 7,116, AV1,AW1,AR1,AA1,DV1,DW1,DR1,DA1,           1-007
     1                       AV2,AW2,AR2,AA2,DV2,DW2,DR2,DA2,           1-008
     2                       AEE,ARC,DEL,ARR,AMP,AZP,AMT,AZT,           1-009
     3                       AT1,DT1                                    1-010
      READ INPUT TAPE 7,118, BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,           1-011
     1                       BB9,B10,B11                                1-012
      IF(INKODE)150,151,150                                             1-013
  150 READ INPUT TAPE 7,125, (HH(I),XX(I),WX(I),I=1,NTT)                1-014
  151 WRITE OUTPUT TAPE 6,103                                           1-015
      WRITE OUTPUT TAPE 6,104,AV1,AW1,AR1,AA1                           1-016
      WRITE OUTPUT TAPE 6,105,DV1,DW1,DR1,DA1                           1-017
      IF(KDGRD)140,141,140                                              1-018
  140 WRITE OUTPUT TAPE 6,144,NV1X,NW1X,NR1X,NA1X                       1-019
  141 WRITE OUTPUT TAPE 6,106,AV2,AW2,AR2,AA2                           1-020
      WRITE OUTPUT TAPE 6,107,DV2,DW2,DR2,DA2                           1-021
      IF(KDGRD)142,143,142                                              1-022
  142 WRITE OUTPUT TAPE 6,145,NV2X,NW2X,NR2X,NA2X                       1-023
  143 WRITE OUTPUT TAPE 6,108,AEE,ARC,DEL,ARR                           1-024
      WRITE OUTPUT TAPE 6,109,AMP,AZP,AMT,AZT                           1-025
      WRITE OUTPUT TAPE 6,110,AT1,DT1,NT1,NTT                           1-026
      WRITE OUTPUT TAPE 6,111,BB1,BB2,BB3,BB4                           1-027
      WRITE OUTPUT TAPE 6,112,BB5,BB6,BB7,BB8                           1-028
      WRITE OUTPUT TAPE 6,113,BB9,B10,B11                               1-029
      WRITE OUTPUT TAPE 6,114,NN1,NN2,NN3,NN4                           1-030
      WRITE OUTPUT TAPE 6,115,NN5,NN6,NN7,NN8                           1-031
      WRITE OUTPUT TAPE 6,160,INKODE,KDPLT,KDGRD,KDCAL                  1-032
      IF(INKODE)153,152,153                                             1-033
  152 DO 154 I=1,NTT                                                    1-034
  154 HH(I)=HS(I)                                                       1-035
      GO TO 156                                                         1-036
  153 DO 155 I=1,NTT                                                    1-037
  155 HS(I)=HH(I)                                                       1-038
      WRITE OUTPUT TAPE 6,117                                           1-039
      WRITE OUTPUT TAPE 6,119,(HH(I),XX(I),WX(I),I=1,NTT)               1-040
  156 CONTINUE                                                          1-041
```

```
  101 FORMAT(13A6)
  102 FORMAT(20H1 ELASTIC SCATTERING/1H013A6)
  103 FORMAT(20H0 INPUT TO PART ONE )
  104 FORMAT(9H0    AV1 =1PE15.8, 9H    AW1 =1PE15.8,
     1        9H    AR1 =1PE15.8, 9H    AA1 =1PE15.8)
  105 FORMAT(9H0    DV1 =1PE15.8, 9H    DW1 =1PE15.8,
     1        9H    DR1 =1PE15.8, 9H    DA1 =1PE15.8)
  144 FORMAT(9H0    NV1 =I15    , 9H    NW1 =I15    ,
     1        9H    NR1 =I15    , 9H    NA1 =I15    )
  106 FORMAT(9H0    AV2 =1PE15.8, 9H    AW2 =1PE15.8,
     1        9H    AR2 =1PE15.8, 9H    AA2 =1PE15.8)
  107 FORMAT(9H0    DV2 =1PE15.8, 9H    DW2 =1PE15.8,
     1        9H    DR2 =1PE15.8, 9H    DA2 =1PE15.8)
  145 FORMAT(9H0    NV2 =I15    , 9H    NW2 =I15    ,
     1        9H    NR2 =I15    , 9H    NA2 =I15    )
  108 FORMAT(9H0    AEF =1PE15.8, 9H    ARC =1PE15.8,
     1        9H    DEL =1PE15.8, 9H    ARR =1PE15.8)
  109 FORMAT(9H0    AMP =1PE15.8, 9H    AZP =1PE15.8,
     1        9H    AMT =1PE15.8, 9H    AZT =1PE15.8)
  110 FORMAT(9H0    AT1 =1PE15.8, 9H    DT1 =1PE15.8,
     1        9H    NT1 =I15    , 9H    NTT =I15    )
  111 FORMAT(9H0    BB1 =1PE15.8, 9H    BB2 =1PE15.8,
     1        9H    BB3 =1PE15.8, 9H    BB4 =1PE15.8)
  112 FORMAT(9H0    BB5 =1PE15.8, 9H    BB6 =1PE15.8,
     1        9H    BB7 =1PE15.8, 9H    BB8 =1PE15.8)
  113 FORMAT(9H0    BB9 =1PE15.8, 9H    B10 =1PE15.8,
     1        9H    B11 =1PE15.8)
  114 FORMAT(9H0    NN1 =I15    , 9H    NN2 =I15    ,
     1        9H    NN3 =I15    , 9H    NN4 =I15    )
  115 FORMAT(9H0    NN5 =I15    , 9H    NN6 =I15    ,
     1        9H    NN7 =I15    , 9H    NN8 =I15    )
  160 FORMAT(9H0INKODE =I15     , 9H KDPLT =I15    ,
     1        9H  KDGRD =I15    , 9H KDCAL =I15    )
  116 FORMAT(8F10.0)
  117 FORMAT(16H1 CM ANGLE (DEG),20H  CROSS SECTION (MB),
     1                          21H  ERROR WEIGHT FACTOR)
  118 FORMAT(8E10.0)
  119 FORMAT(0PF16.3,1P2E20.8)
  120 FORMAT(15I5)
  125 FORMAT(6F10.0)
C     REDUCED MASS
      X=(AMP*AMT)/(AMP+AMT)
C     WAVE NUMBER
      AEE = AEE*X/AMP
      AKS = (2.0*X*AEE)/41.826134
      AKK = SQRTF(AKS)
C     MESH SIZE
      ADD=1000.0*DEL/AKK
      ADD=0.001*INTF(ADD+0.5)
C     COULOMB PARAMETER
      AZZ=(AZP*AZT*X*0.034444017)/AKK
      A2D=2.0*ADD
      A3D=3.0*ADD
      A6D=6.0*ADD
C     NORMALIZATION FACTOR FOR L=0 RADIAL WAVE FUNCTION
      IF(AZZ) 121,122,121
  122 ACC=1.0
      GO TO 123
  121 Y=6.2831853*AZZ
      ACC=SQRTF(Y/(EXPF(Y)-1.0))
C     INTERVAL DOUBLING RADIUS
```

```
  123 IRR=ARR/A3D+0.50
      IRR=3*IRR
      ARR=ADD*FLOATF(IRR)
C     MAXIMUM RADIUS
      Y=ARR+12.0*ADD
      X=AR1+AA1*BB1+BB2
      Z=AR2+AA2*BB1+BB2
      W=BB3+AZZ/AKK
      ARM=MAX1F(X,Y,Z,W)
      IRM=(ARM-ARR)/A6D+0.50
      IRM=3*IRM
      ARM=ARR+A2D*FLOATF(IRM)
      IRM=IRR+IRM
      D12=ADD*ADD/12.0
C     MAXIMUM L VALUE
      LRM=AKK*ARM+BB4
      LRM=XMINOF(LRM,50)
      DDS=D12*AKS/AEF
      X=AZZ*AZZ
C     NORMALIZATION FACTORS FOR RADIAL WAVE FUNCTION
      DO 124 I=1,LRM
      Y=I
  124 QQ(I)=SQRTF(Y*Y+X)/(Y*(2.0*Y+1.0))
      WRITE OUTPUT TAPE 6,131
      WRITE OUTPUT TAPE 6,132,AKK,ADD,AZZ,ACC
      WRITE OUTPUT TAPE 6,133,ARR,ARM,IRR,IRM
      WRITE OUTPUT TAPE 6,134,LRM
  131 FORMAT(21H1 OUTPUT FROM PROGRAM)
  132 FORMAT(9H0    AKK =1PE15.8, 9H     ADD =1PE15.8,
     1        9H    AZZ =1PE15.8, 9H     ACC =1PE15.8)
  133 FORMAT(9H0    ARR =1PE15.8, 9H     ARM =1PE15.8,
     1        9H    IRR =I15,     9H     IRM =I15     )
  134 FORMAT(9H0    LRM =I15 )
C     PREPARATION FOR PROGRAM EIGHT
      II4=NN6
      K800=0
      RETURN
      END
```

```
      SUBROUTINE TWO                                                    2-000
C     PROGRAM TWO    COULOMB PHASE SHIFTS AND WAVE FUNCTIONS            2-001
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,    C-01
     1       AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                            C-02
     2       BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,      C-03
     3       CC,CN,CS,                                                   C-04
     4       DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,             C-05
     5       ERR,FF,GG,HH,HS,                                            C-06
     6       II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                     C-07
     7       KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,             C-08
     8       LL,LLM,LRM,                                                 C-09
     9       NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X     C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                     C-11
     1       QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                         C-12
      DIMENSION BM(51),BP(51),                                           D-01
     1          CC(2,100),CN(90),CS(51),                                 D-02
     2          DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),        D-03
     3          QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),   D-04
     4          WW(500),WX(90),                                          D-05
     5          XC(90),XN(90),XX(90)                                     D-06
      DIMENSION AA(100),AS(51),BB(100),FA(2,101)                         D-07
C     COULOMB PHASE SHIFTS                                              2-002
      A=ATANF(AZZ/51.0)                                                 2-003
      B=SQRTF(2601.0+AZZ**2)                                            2-004
C     STIRLINGS FORMULA GIVES AS (L+1) FOR LARGE L                      2-005
      AS(51)=50.5*A+AZZ*LOGF(B)-AZZ-SINF(A)/(12.0*B)+SINF(3.            2-006
     1 0*A)/(360.0*B**3)-SINF(5.0*A)/(1260.0*B**5)+SINF(7.0*A)/(1680    2-007
     2 .0*B**7)                                                         2-008
       DO 201 I=1,50                                                    2-009
       J=51-I                                                           2-010
  201 AS(J)=AS(J+1)-ATANF(AZZ/FLOATF(J))                                2-011
      ASS=2.0*AS(1)+AZZ*0.69314718                                      2-012
      DO 202 I=1,51                                                     2-013
      A=2.0*AS(I)                                                       2-014
      CS(I)=COSF(A)                                                     2-015
  202 SN(I)=SINF(A)                                                     2-016
C     COULOMB WAVE FUNCTIONS FOR L=0,1 BY ASYMPTOTIC SERIES             2-017
  203 DO 204 M=1,2                                                      2-018
      DO 205 N=1,2                                                      2-019
      L=M-1                                                             2-020
      R=ARM+A2D*FLOATF(N-2)                                             2-021
      A=2.0*AZZ                                                         2-022
      T=L                                                               2-023
      B=T*(T+1.0)+AZZ*AZZ                                               2-024
      C=2.0*R*AKK                                                       2-025
      U=1.0                                                             2-026
      V=0.0                                                             2-027
      X=1.0                                                             2-028
      Y=0.0                                                             2-029
      DO 206 J=1,NN1                                                    2-030
      D=J                                                               2-031
      P=(A-AZZ/D)/C                                                     2-032
      Q=(B/D+1.0-D)/C                                                   2-033
      ZR=X*P - Y*Q                                                      2-034
      ZI=X*Q + Y*P                                                      2-035
      DIV= ZR*ZR + ZI*ZI - X*X - Y*Y                                    2-036
      IF(DIV)230,207,207                                                2-037
  230 X=ZR                                                              2-038
      Y=ZI                                                              2-039
      U=U+X                                                             2-040
      V=V+Y                                                             2-041
```

```
      Z=(X**2+Y**2)/(U**2+V**2)
      IF(Z-BB5) 207,206,206
  206 CONTINUE
      GO TO 209
  207 P=R*AKK-AZZ*LOGF(C)+AS(L+1)-1.5707963*T
      X=COSF(P)
      Y=SINF(P)
      FF(N,M)=X*V+Y*U
  205 GG(N,M)=X*U-Y*V
  204 CONTINUE
C     CHECK ACCURACY OF RESULT WITH WRONSKIAN RELATION
      A=1.0/SQRTF(1.0+AZZ**2)
      B=FF(1,1)*GG(1,2)-FF(1,2)*GG(1,1)-A
      C=FF(2,1)*GG(2,2)-FF(2,2)*GG(2,1)-A
      B=ABSF(B)
      C=ABSF(C)
      IF(B-1.E-5)2081,209,209
 2081 IF(C-1.E-5)208,209,209
  209 ARM=ARM+A6D*FLOATF(NN2)
      IRM=IRM+3*NN2
      IF(IRM-500)203,260,260
  260 WRITE OUTPUT TAPE 6,240
  240 FORMAT(68H0 ARM EXCEEDS AVAILABLE STORAGE FOR POTENTIALS, PROCEED
     1TO NEXT CASE)
      IF(KDPLT)261,262,261
  261 READ INPUT TAPE 7,241,PLOT
  241 FORMAT(F10.0)
  262 KODE2=1
      RETURN
C     COULOMB WAVE FUNCTIONS FOR L MORE THAN 1 BY RECURRENCE RELATIONS
C     GET COEFFICIENTS FOR THE RECURRENCE RELATIONS
  208 L=LRM+10
      DO 210 I=1,L
      BB(I)=AZZ/FLOATF(I)
  210 AA(I)=SQRTF(1.0+BB(I)**2)
      J=L-1
      DO 211 N=1,2
      R=AKK*(ARM+A2D*FLOATF(N-2))
      DO 212 I=1,J
  212 CC(N,I)=FLOATF(2*I+1)/R+BB(I)+BB(I+1)
  211 CONTINUE
C     RECURR UP TO GET THE IRREGULAR COULOMB WAVE FUNCTIONS
      J=LRM+1
      DO 213 N=1,2
      DO 214 I=3,J
  214 GG(N,I)=(CC(N,I-2)*GG(N,I-1)-AA(I-2)*GG(N,I-2))/AA(I-1)
  213 CONTINUE
C     RECURR DOWN TO GET THE REGULAR COULOMB WAVE FUNCTIONS
  215 J=L+1
      FA(1,J)=0.0
      FA(2,J)=0.0
      FA(1,L)=0.1
      FA(2,L)=0.1
      K=L-1
      DO 216 N=1,2
      DO 217 I=1,K
      J=L-I
      FA(N,J)=(CC(N,J)*FA(N,J+1)-AA(J+1)*FA(N,J+2))/AA(J)
      IF(FA(N,J)-1.E30) 217,231,231
  231 IF(J-LRM+1) 232,233,233
  233 FA(N,J)=FA(N,J)*1.E-30
```

```
      FA(N,J+1)=FA(N,J+1)*1.E-30
      GO TO 217
  232 JK=LRM+1
      DO 234 IJ=J,JK
  234 FA(N,IJ)=FA(N,IJ)*1.E-30
  217 CONTINUE
  216 CONTINUE
C     RENORMALIZE THE REGULAR COULOMB WAVE FUNCTIONS
      C=FF(1,1)/FA(1,1)
      D=FF(2,1)/FA(2,1)
      DO 218 I=1,L
      FA(1,I)=C*FA(1,I)
  218 FA(2,I)=D*FA(2,I)
C     CHECK ALL COULOMB WAVE FUNCTIONS WITH WRONSKIAN RELATION
      M=LRM+1
      DO 219 I=3,M
      D=FA(1,I-1)*GG(1,I)-FA(1,I)*GG(1,I-1)-1.0/AA(I-1)
      IF(ABSF(D)-1.E-5)219,219,221
  219 CONTINUE
      GO TO 220
C     RECURRENCE RELATION HAS FAILED    INCREASE L AND TRY AGAIN
  221 J=L+1
      L=L+10
      IF(L-100)222,222,223
  223 WRITE OUTPUT TAPE 6,229
  229 FORMAT(74HORECURRENCE RELATIONS FOR COULOMB WAVE FUNCTION HAVE FAI
     1LED, INCREASE RMAX/)
      GO TO 209
  222 DO 224 I=J,L
C     ADDITIONAL COEFFICIENTS FOR THE  RECURSION RELATIONS
      BB(I)=AZZ/FLOATF(I)
  224 AA(I)=SQRTF(1.0+BB(I)**2)
      M=J-1
      K=L-1
      LLM=K
      DO 225 N=1,2
      R=AKK*(ARM+A2D*FLOATF(N-2))
      DO 226 I=M,K
  226 CC(N,I)=FLOATF(2*I+1)/R+BB(I)+BB(I+1)
  225 CONTINUE
      GO TO 215
  220 DO 228 N=1,2
      DO 227 I=1,51
  227 FF(N,I)=FA(N,I)
  228 CONTINUE
  250 FORMAT(15H0   FINAL VALUE 5X,5HARM =1PE15.8,5X,5HIRM =I4)
      WRITE OUTPUT TAPE 6,250,ARM,IRM
      KODE2=2
      RETURN
      END
```

```
      SUBROUTINE THREE
C     PROGRAM THREE    COULOMB POTENTIAL AND R SQUARED
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,
     1       AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,
     2       BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,
     3       CC,CN,CS,
     4       DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,
     5       ERR,FF,GG,HH,HS,
     6       II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,
     7       KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,
     8       LL,LLM,LRM,
     9       NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,
     1       QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX
      DIMENSION BM(51),BP(51),
     1          CC(2,100),CN(90),CS(51),
     2          DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),
     3          QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),
     4          WW(500),WX(90),
     5          XC(90),XN(90),XX(90)
C     PUT RC ON THE MESH
      R = ARC - ARR
      IF(R) 301,301,302
  301 I=ARC/A3D+0.5
      J=3*I
      ARC=ADD*FLOATF(J)
      GO TO 303
  302 I=R/A6D+0.5
      J=3*I
      ARC=ARR+A2D*FLOATF(J)
      J=IRR+J
  303 WRITE OUTPUT TAPE 6,304,ARC,J
  304 FORMAT(15H0   FINAL VALUE5X,5HARC =1PE15.8,5X,5HIRC =I4//)
      ICC=J
C     CALCULATE THE COULOMB POTENTIAL
      AZD=2.0*AKK*AZZ
      W=D12*AZD
      X=D12*AKS
      Y=W*1.5/ARC
      Z=Y*0.33333333/(ARC**2)
      Y=X-Y
      R=0.0
      K=XMINOF(J,IRR)
      DO 305 I=1,K
      R=R+ADD
      RR(I)=R*R
  305 VC(I)=Y+Z*RR(I)
      IF(J-IRR) 306,307,308
  306 K=J+1
      DO 309 I=K,IRR
      R=R+ADD
      RR(I)=R*R
  309 VC(I)=X-W/R
      K=IRR+1
      X=4.0*X
      W=4.0*W
      GO TO 310
  308 K=IRR+1
      Y=4.0*Y
      Z=4.0*Z
      DO 311 I=K,J
      R=R+A2D
      RR(I)=R*R
  311 VC(I)=Y+Z*RR(I)
  307 K=J+1
      W=4.0*W
      X=4.0*X
  310 DO 312 I=K,IRM
      R=R+A2D
      RR(I)=R*R
  312 VC(I)=X-W/R
      RETURN
      END
```

```
      SUBROUTINE FOUR                                                   4-000
C     PROGRAM FOUR     OPTICAL POTENTIAL FORM FACTORS AND POWER SERIES  4-001
C                      COEFFICIENTS                                     4-002
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,    C-01
     1       AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                            C-02
     2       BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,      C-03
     3       CC,CN,CS,                                                   C-04
     4       DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,             C-05
     5       ERR,FF,GG,HH,HS,                                            C-06
     6       II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                     C-07
     7       KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,             C-08
     8       LL,LLM,LRM,                                                 C-09
     9       NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X     C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                     C-11
     1       QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                         C-12
      DIMENSION BM(51),BP(51),                                           D-01
     1          CC(2,100),CN(90),CS(51),                                 D-02
     2          DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),        D-03
     3          QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),   D-04
     4          WW(500),WX(90),                                          D-05
     5          XC(90),XN(90),XX(90)                                     D-06
      DIMENSION AC(100)                                                  D-07
C     CALCULATION OF SAXON FORM FACTOR                                  4-003
  401 A=EXPF(ADD/AA1)                                                   4-004
      B=EXPF(-AR1/AA1)                                                  4-005
      DO 402 I=1,IRR                                                    4-006
      B=B*A                                                             4-007
  402 SS(I)=1.0/(1.0+B)                                                 4-008
      A=A*A                                                             4-009
      J=IRR+1                                                           4-010
      DO 403 I=J,IRM                                                    4-011
      B=B*A                                                             4-012
      SS(I)=1.0/(1.0+B)                                                 4-013
      IF(SS(I)-BB6) 404,403,403                                         4-014
  403 CONTINUE                                                          4-015
      GO TO 405                                                         4-016
  404 NNN=XMAXOF(I,IRR+6)                                               4-017
      J=I+1                                                             4-018
      DO 406 I=J,IRM                                                    4-019
  406 SS(I)=0.0                                                         4-020
      GO TO 407                                                         4-021
  405 NNN=IRM+1                                                         4-022
  407 IF(NN3) 408,409,408                                               4-023
C     CALCULATION OF SURFACE INTERACTION FORM FACTOR                    4-024
  408 X=ADD/AA2                                                         4-025
      Y=-AR2/AA2                                                        4-026
      Z=LOGF(BB6)                                                       4-027
      DO 410 I=1,IRR                                                    4-028
      Y=Y+X                                                             4-029
      IF(Y-Z) 410,412,412                                               4-030
  410 TT(I)=0.0                                                         4-031
      GO TO 413                                                         4-032
  412 NTN=I                                                             4-033
      Y=EXPF(Y-X)                                                       4-034
      X=EXPF(X)                                                         4-035
      DO 414 J=I,IRR                                                    4-036
      Y=Y*X                                                             4-037
  414 TT(J)=4.0/(2.0+Y+1.0/Y)                                           4-038
      X=X*X                                                             4-039
      J=IRR+1                                                           4-040
  415 DO 416 I=J,IRM                                                    4-041
```

```
      II=I
      Y=Y*X
      TT(I)=4.0/(2.0+Y+1.0/Y)
      IF(TT(I)-BB6) 417,416,416
  416 CONTINUE
      I=II
  417 NNN=XMAXOF(NNN,I)
      IF(I-IRM) 418,409,418
  418 K=I+1
      DO 420 J=K,IRM
  420 TT(J)=0.0
      GO TO 409
  413 X=2.0*X
      J=IRR+1
      DO 422 I=J,IRM
      Y=Y+X
      IF(Y-Z) 422,423,423
  422 TT(I)=0.0
      GO TO 409
  423 NTN=I
      Y=EXPF(Y-X)
      X=EXPF(X)
      J=I
      GO TO 415
  409 A=NNN-IRR
      N3N=A/6.+.5
      NNN=IRR+3*N3N
      I3I=(IRM-NNN)/3
C     CALCULATION OF POWER SERIES COEFFICIENTS
C     FIRST CALCULATE THE SAXON WELL COEFFICIENTS
      A=EXPF(-AR1/AA1)
      CC(1,1)=1.0/(1.0+A)
      B=-A*CC(1,1)
      AC(1)=1.0
      CC(1,2)=-A*CC(1,1)**2/AA1
      AC(2)=1.0
      D=CC(1,1)/(2.0*AA1*AA1)
      CC(1,3)=CC(1,1)*CC(1,2)*(1.0-A)/(2.0*AA1)
      DO 451 I=3,NN4
      AC(I)=1.0
      DO 452 J=3,I
      K=I+2-J
  452 AC(K)=AC(K)*FLOATF(K)+AC(K-1)
      K=I+1
      D=D/(AA1*FLOATF(I))
      IF(D-1.E-30) 463,463,464
  464 E=1.
      F=0.0
      DO 453 J=1,I
      E=E*B*FLOATF(J)
      IF(ABSF(E)-1.E-30) 461,461,453
  461 E=0.
  453 F=F+AC(J)*E
  451 CC(1,K)=F*D
  463 DO 467 II=K,LLM
  467 CC(1,II)=0.
  459 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE FIVE                                                   5-000
C     PROGRAM FIVE      THE EFFECTIVE KINETIC ENERGY  AND COMBINED      5-001
C                       POWER SERIES COEFFICIENTS                       5-002
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,    C-01
     1       AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                            C-02
     2       BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,      C-03
     3       CC,CN,CS,                                                   C-04
     4       DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,             C-05
     5       ERR,FF,GG,HH,HS,                                            C-06
     6       II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                     C-07
     7       KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,             C-08
     8       LL,LLM,LRM,                                                 C-09
     9       NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X     C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                     C-11
     1       QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                         C-12
      DIMENSION BM(51),BP(51),                                           D-01
     1          CC(2,100),CN(90),CS(51),                                 D-02
     2          DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),        D-03
     3          QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),   D-04
     4          WW(500),WX(90),                                          D-05
     5          XC(90),XN(90),XX(90)                                     D-06
C     CONTRIBUTION TO E.K.E. DUE TO K.E., SAXON POTENTIAL, AND          5-003
C      COULOMB POTENTIAL                                                5-004
  500 V=-AV1*DDS                                                        5-005
      W=-AW1*DDS                                                        5-006
      DO 501 I=1,IRR                                                    5-007
      VV(I)=VC(I)-V*SS(I)                                               5-008
  501 WW(I)=-W*SS(I)                                                    5-009
      J=IRR+1                                                           5-010
      V=4.0*V                                                           5-011
      W=4.0*W                                                           5-012
      DO 502 I=J,NNN                                                    5-013
      VV(I)=VC(I)-V*SS(I)                                               5-014
  502 WW(I)=-W*SS(I)                                                    5-015
      J=NNN+1                                                           5-016
      DO 503 I=J,IRM                                                    5-017
      WW(I)=0.0                                                         5-018
  503 VV(I)=VC(I)                                                       5-019
      IF(NN3) 505,504,505                                               5-020
C     CONTRIBUTION TO E.K.E. DUE TO SURFACE INTERACTION POTENTIAL       5-021
  505 V=-AV2*DDS                                                        5-022
      W=-AW2*DDS                                                        5-023
      IF(NTN-IRR) 507,507,508                                           5-024
  507 DO 506 I=NTN,IRR                                                  5-025
      VV(I)=VV(I)-V*TT(I)                                               5-026
  506 WW(I)=WW(I)-W*TT(I)                                               5-027
      GO TO 516                                                         5-028
  508 J=NTN                                                             5-029
      GO TO 515                                                         5-030
  516 J=IRR+1                                                           5-031
  515 V=4.0*V                                                           5-032
      W=4.0*W                                                           5-033
      DO 509 I=J,NNN                                                    5-034
      VV(I)=VV(I)-V*TT(I)                                               5-035
  509 WW(I)=WW(I)-W*TT(I)                                               5-036
C     CALCULATE COMBINED POWER SERIES COEFFICIENTS                      5-037
  504 A=-DDS/D12                                                        5-038
      S=-A*AV1                                                          5-039
      T=-A*AW1                                                          5-040
  511 DO 514 I=1,NN4                                                    5-041
      DD(1,I)=S*CC(1,I)                                                 5-042
  514 DD(2,I)=T*CC(1,I)                                                 5-043
  513 CONTINUE                                                          5-044
      RETURN                                                            5-045
      END                                                               5-046
```

```
      SUBROUTINE SIX                                                    6-000
C     PROGRAM SIX    THE RADIAL WAVE FUNCTIONS AND ASSOCIATED SCATTERING  6-001
C                    AMPLITUDES                                         6-002
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,    C-01
     1       AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                            C-02
     2       BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,      C-03
     3       CC,CN,CS,                                                   C-04
     4       DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,             C-05
     5       ERR,FF,GG,HH,HS,                                            C-06
     6       II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                     C-07
     7       KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,             C-08
     8       LL,LLM,LRM,                                                 C-09
     9       NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X     C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                     C-11
     1       QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                         C-12
      DIMENSION BM(51),BP(51),                                           D-01
     1          CC(2,100),CN(90),CS(51),                                 D-02
     2          DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),        D-03
     3          QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),   D-04
     4          WW(500),WX(90),                                          D-05
     5          XC(90),XN(90),XX(90)                                     D-06
      DIMENSION BB(2,100)                                                D-07
  600 P=0.0                                                             6-003
      MMM=0                                                             6-004
      ICC=ICC                                                           6-005
C     GET STARTING VALUE FOR I                                          6-006
      LL=0                                                              6-007
  601 Q=(2.*P+1.)                                                       6-008
      I3J=I3I                                                           6-009
      R=B11*P*ADD                                                       6-010
  615 RT=P*ADD/3.5                                                      6-011
      IF(R-RT)614,651,651                                               6-012
  651 S=(ABSF(R-ARR) + (R-ARR))/2.0                                     6-013
      IF(S) 602,602,603                                                 6-014
  602 I=R/A3D+0.5                                                       6-015
      I=XMAXOF(I,1)                                                     6-016
      I=3*I                                                             6-017
      R=ADD*FLOATF(I)                                                   6-018
      GO TO 604                                                         6-019
  603 I=S/A6D+0.5                                                       6-020
      I=3*I                                                             6-021
      R=ARR+A2D*FLOATF(I)                                               6-022
      I=IRR+I                                                           6-023
C     INITIAL MESH SIZE                                                 6-024
  604 IF(I-IRR) 605,606,606                                             6-025
  605 E=ADD                                                             6-026
      L=1                                                               6-027
      GO TO 607                                                         6-028
  606 E=A2D                                                             6-029
      L=2                                                               6-030
  607 IF(R-ARC) 608,608,609                                             6-031
  608 X=0.0                                                             6-032
      Y=1.0                                                             6-033
      GO TO 610                                                         6-034
  609 X=1.0                                                             6-035
      Y=0.0                                                             6-036
C     GET FIRST COUPLE TERMS OF POWER SERIES                            6-037
  610 B=1.5*AZD*Y/ARC                                                   6-038
      C=X*AZD                                                           6-039
      A=B-AKS                                                           6-040
      S=R-E                                                             6-041
```

```
      B=0.33333333*B/RR(ICC)
      BB(1,1)=1.0
      BB(2,1)=0.0
      BB(1,2)=C/(Q+1.0)
      BB(2,2)=0.0
      T=2.0*(Q+2.0)
      BB(1,3)=(A-DD(1,1)+C*BB(1,2))/T
      F=R*R
      G=S*S
      Z=F*R
      W=G*S
      BB(2,3)=(-DD(2,1)/T)
      T=3.0*(Q+3.0)
      BB(1,4)=(-DD(1,2)+C*BB(1,3)+A*BB(1,2)-DD(1,1)*BB(1,2))/T
      BB(2,4)=(-DD(2,2)+C*BB(2,3)-DD(2,1)*BB(1,2))/T
      X=BB(1,1)+BB(1,3)*F+BB(1,4)*Z+BB(1,2)*R
      U=BB(1,1)+BB(1,3)*G+BB(1,4)*W+BB(1,2)*S
      Y=BB(2,3)*F+BB(2,4)*Z
  650 V=BB(2,3)*S+BB(2,4)*W
C     GET ADDITIONAL TERMS TO POWER SERIES BY RECURSION
      DO 611  N=5,NN4
      W=W*S
      Z=Z*R
      T=N-1
      T=T*(T+Q)
      G=0.0
      K=N-2
      H=0.0
      DO 612 J=1,K
      M=N-J-1
      G=G+DD(1,J)*BB(1,M)-DD(2,J)*BB(2,M)
  612 H=H+DD(1,J)*BB(2,M)+DD(2,J)*BB(1,M)
      BB(1,N)=(A*BB(1,N-2)-B*BB(1,N-4)-G+C*BB(1,N-1))/T
      BB(2,N)=(A*BB(2,N-2)-B*BB(2,N-4)-H+C*BB(2,N-1))/T
      G=BB(1,N)*Z
      H=BB(2,N)*Z
      X=X+G
      Y=Y+H
      U=U+BB(1,N)*W
      V=V+BB(2,N)*W
      IF(XMODF(N,2))639,640,639
  639 IF(NN8-N)613,613,640
  640 F=(G**2+H**2)/(X**2+Y**2)
      IF(F-BB7) 613,611,611
  611 CONTINUE
      R=R-6.0*E
      MMM=MMM+1
      IF(R-A3D) 614,615,615
  614 WRITE OUTPUT TAPE 6,641,MMM,P
  641 FORMAT(39H0POWER SERIES FAILED TO CONVERGE IN SIX/5H0MMM=I5,5X,2HP
     1=F10.6)
      IF(KDPLT)661,662,661
  661 READ INPUT TAPE 7,663,PLOT
  663 FORMAT(F10.0)
  662 KODE6=1
      RETURN
C     NORMALIZE WAVE FUNCTIONS
  613 A=AKK*R
      B=AKK*S
      F=A*ACC
      G=B*ACC
```

```
      IF(LL) 616,616,617
  617 DO 618 K=1,LL
      F=F*A*QQ(K)
  618 G=G*B*QQ(K)
  616 U=U*G
      V=V*G
      X=X*F
      Y=Y*F
C     NOW INTEGRATE THE DIFF EQUATION
C     SET UP INITIAL VALUES
      H=D12*P*(P+1.0)
      F=1.0+VV(I)-H/RR(I)
      G=WW(I)
      JJ=I-L
      C=1.0+VV(JJ)-H/RR(JJ)
      D=WW(JJ)
      ASSIGN 622 TO II
      IF(L-1) 619,619,620
  619 J=(IRR-I)/3
C     INTEGRATION WITH A COMPLEX POTENTIAL
  624 DO 621 K=1,J
      I=I+1
      A=1.0+VV(I)-H/RR(I)
      B=WW(I)
      Z=A*A+B*B
      Q=12.0-10.0*F
      XP=(Q*X-C*U+10.0*G*Y+D*V)
      XM=(Q*Y-C*V-10.0*G*X-D*U)
      S=(A*XP+B*XM)/Z
      T=(A*XM-B*XP)/Z
      I=I+1
      C=1.0+VV(I)-H/RR(I)
      D=WW(I)
      Z=C*C+D*D
      Q=12.0-10.0*A
      XP=(Q*S-F*X+10.0*B*T+G*Y)
      XM=(Q*T-F*Y-10.0*B*S-G*X)
      U=(C*XP+D*XM)/Z
      V=(C*XM-D*XP)/Z
      I=I+1
      F=1.0+VV(I)-H/RR(I)
      G=WW(I)
      Z=F*F+G*G
      Q=12.0-10.0*C
      XP=(Q*U-A*S+10.0*D*V+B*T)
      XM=(Q*V-A*T-10.0*D*U-B*S)
      X=(F*XP+G*XM)/Z
  621 Y=(F*XM-G*XP)/Z
      GO TO II,(622,623)
C     CHANGE OF INTERVAL SIZE
  622 U=S
      J=N3N
      V=T
      F=4.0*F-3.0
      C=4.0*A-3.0
      G=4.0*G
      D=4.0*B
      GO TO 626
  620 J=(NNN-I)/3
  626 ASSIGN 623 TO II
      H=4.0*H
```

```
      IF(J)631,623,624
  631 I3J=I3I+J
      IF(I3J)627,632,623
C     INTEGRATION WITH A REAL POTENTIAL
  623 DO 625 K=1,I3J
      I=I+1
      A=1.0+VV(I)-H/RR(I)
      Q=12.0-10.0*F
      S=(Q*X-C*U)/A
      T=(Q*Y-C*V)/A
      I=I+1
      C=1.0+VV(I)-H/RR(I)
      Q=12.0-10.0*A
      U=(Q*S-F*X)/C
      V=(Q*T-F*Y)/C
      I=I+1
      F=1.0+VV(I)-H/RR(I)
      Q=12.0-10.0*C
      X=(Q*U-A*S)/F
  625 Y=(Q*V-A*T)/F
C     CALCULATION OF THE SCATTERING AMPLITUDES
  632 LL=LL+1
      A=X*FF(1,LL)-U*FF(2,LL)
      B=Y*FF(1,LL)-V*FF(2,LL)
      C=X*GG(1,LL)-U*GG(2,LL)
      D=Y*GG(1,LL)-V*GG(2,LL)
      E=(A+D)**2+(B-C)**2
      BP(LL)=(((D+A)*(D-A)+(C+B)*(C-B))/E)-1.0
      BM(LL)=(-2.0)*(A*C+B*D)/E
C     SHALL WE GO AROUND AGAIN
      IF(ABSF(BP(LL)) + ABSF(BM(LL)) - BB8 ) 627,628,628
  628 IF(LL-LRM) 629,629,627
  629 P=P+1.0
      GO TO 601
  630 FORMAT(9H0    MMM =I15,9H    LRM =I15,9H   LMAX =5X,2PE10.3)
  627 WRITE OUTPUT TAPE 6,630,MMM,LRM,P
      KODE6=2
      RETURN
      END
```

```
      SUBROUTINE SEVEN                                                  7-000
C     PROGRAM SEVEN    THE ELASTIC CROSS SECTION                        7-001
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,    C-01
     1       AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                            C-02
     2       BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,      C-03
     3       CC,CN,CS,                                                   C-04
     4       DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,             C-05
     5       ERR,FF,GG,HH,HS,                                            C-06
     6       II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                     C-07
     7       KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,             C-08
     8       LL,LLM,LRM,                                                 C-09
     9       NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X     C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                     C-11
     1       QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                         C-12
      DIMENSION BM(51),BP(51),                                           D-01
     1          CC(2,100),CN(90),CS(51),                                 D-02
     2          DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),        D-03
     3          QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),   D-04
     4          WW(500),WX(90),                                          D-05
     5          XC(90),XN(90),XX(90)                                     D-06
  736 IF(NN5) 708,708,732                                               7-002
  732 KODE7=2                                                           7-003
  719 ASSIGN 702 TO KK                                                  7-004
      ASSIGN 717 TO JJ                                                  7-005
      ERR=0.0                                                           7-006
      N=NTT                                                             7-007
  706 DO 701 J=1,N                                                      7-008
      X=COSF(HH(J)*0.017453293)                                         7-009
      A=(1.0-X)                                                         7-010
      B=AZZ/A                                                           7-011
      C=ASS-AZZ*LOGF(A)                                                 7-012
      E=-B*COSF(C)                                                      7-013
      F=-B*SINF(C)                                                      7-014
      PL(1)=1.0                                                         7-015
      PL(2)=X                                                           7-016
      G=0.5*(BP(1)*SN(1)+BM(1)*CS(1))+1.5*X*(BP(2)*SN(2)+BM(2)*CS(2))   7-017
      H= 0.5*(BM(1)*SN(1)-BP(1)*CS(1))+1.5*X*(BM(2)*SN(2)-BP(2)*CS(2))  7-018
      DO 718 K=3,LL                                                     7-019
      D=K-1                                                             7-020
      PL(K)=((2.0*D-1.0)*X*PL(K-1)-(D-1.0)*PL(K-2))/D                   7-021
      A=PL(K)*(D+0.5)                                                   7-022
      G=G+A*(BP(K)*SN(K)+BM(K)*CS(K))                                   7-023
  718 H=H+A*(BM(K)*SN(K)-BP(K)*CS(K))                                   7-024
      XN(J)=((E+G)**2+(F+H)**2)*10.0/AKS                                7-025
      GO TO KK,(702,713)                                                7-026
  713 XC(J)=(E**2+F**2)*10.0/AKS                                        7-027
      IF(XC(J))721,720,721                                              7-028
  720 CN(J)=0.                                                          7-029
      GO TO 722                                                         7-030
  721 CN(J)=XN(J)/XC(J)                                                 7-031
  722 CONTINUE                                                          7-032
      WRITE OUTPUT TAPE 6,711,HH(J),XN(J),XC(J),CN(J)                   7-033
      GO TO 701                                                         7-034
  702 ERR=ERR+WX(J)*((XN(J)-XX(J))/XX(J))**2                            7-035
  701 CONTINUE                                                          7-036
      GO TO JJ, (717,715)                                               7-037
  703 FORMAT(9H    AV1 =1PE15.8, 9H    AW1 =1PE15.8,                    7-038
     1       9H    AR1 =1PE15.8, 9H    AA1 =1PE15.8)                    7-039
  704 FORMAT(9H    AV2 =1PE15.8, 9H    AW2 =1PE15.8,                    7-040
     1       9H    AR2 =1PE15.8, 9H    AA2 =1PE15.8)                    7-041
  705 FORMAT(9H  ERROR =1PE15.8)                                        7-042
```

```
717 WRITE OUTPUT TAPE 6,703,AV1,AW1,AR1,AA1
    WRITE OUTPUT TAPE 6,704,AV2,AW2,AR2,AA2
    WRITE OUTPUT TAPE 6,705,ERR
    RETURN
710 FORMAT(45H1 CALCULATED VALUES OF ELASTIC CROSS SECTIONS
  1       /16H0 CM ANGLE (DEG),18H    EL XSCTN (MB)
  2        18H   COUL XSCTN (MB) ,18H    EL/COUL
711 FORMAT(F16.3,1PE18.8,1PE18.8,1PE18.8)
708 IF(KDGRD) 731,730,731
731 KODE7=3
    GO TO 719
730 ASSIGN 713 TO KK
    ASSIGN 715 TO JJ
    WRITE OUTPUT TAPE 6,716
    WRITE OUTPUT TAPE 6,703,AV1,AW1,AR1,AA1
    WRITE OUTPUT TAPE 6,704,AV2,AW2,AR2,AA2
    WRITE OUTPUT TAPE 6,705,ERR
716 FORMAT(24H  FINAL PARAMETER VALUES)
    WRITE OUTPUT TAPE 6,710
    IF(KDCAL)751,750,751
750 N=NTT
    NT1=NTT
    KODE7=1
    GO TO 706
751 HH(1)=AT1
    DO 714 I=2,NT1
714 HH(I)=HH(I-1)+DT1
    N=NT1
    KODE7=1
    GO TO 706
715 IF (KDPLT) 733,734,733
733 CALL PLOT7(HS,XX,NTT,HH,XN,NT1,KDCAL)
734 RETURN
    END
```

```
      SUBROUTINE PLOT7(HS,XX,NTT,HH,XN,NT1,KDCAL)
C     CALLING PROGRAM FOR PLOT ROUTINE
      DIMENSION HS(90),XS(90),HH(90),XX(90),XN(90),X(180),Y(180)
      DIMENSION P(11),K(14)
      C=2.3025851
      DO 1 I=1,NTT
    1 XS(I)=-LOGF(XX(I))/C
      DO 2 I=1,NT1
    2 XN(I)=-LOGF(XN(I))/C
C     SET UP CONDITIONS TO ENTER PLOT SUBROUTINE
      P(1)=5.
      READ INPUT TAPE 7,100,(P(I),I=6,11)
      K(1)=48
      K(2)=2
      K(3)=NTT
      K(5)=NT1
      DO 3 I=1,NTT
      X(I)=XS(I)
    3 Y(I)=HS(I)
      DO 4 I=1,NT1
      J=NTT+I
      X(J)=XN(I)
    4 Y(J)=HH(I)
      IF(KDCAL)5,6,5
    5 WRITE OUTPUT TAPE 6,103
  103 FORMAT(49HPTPLOT OF ELASTIC CROSS SECTION VS CM ANGLE (DEG),
     1 5X,58HNOTE - EXPERIMENTAL AND CALCULATED ANGLES ARE NOT THE SAME)
      GO TO 7
    6 WRITE OUTPUT TAPE 6,105
  105 FORMAT(49HPTPLOT OF ELASTIC CROSS SECTION VS CM ANGLE (DEG),
     1 5X,54HNOTE - EXPERIMENTAL AND CALCULATED ANGLES ARE THE SAME)
    7 CALL PLOTMY(X,Y,K,P)
      WRITE OUTPUT TAPE 6,104
  104 FORMAT(16HPL* EXPERIMENTAL5X,14H  + CALCULATED)
  100 FORMAT(6F10.0)
      RETURN
      END
```

```
      SUBROUTINE EIGHT                                                  8-000
C     PROGRAM EIGHT    SEARCHING PROCEDURE                              8-001
      COMMON AA1,AA2,ACC,ADD,AKK,AKS,ARC,ARM,ARR,AR1,AR2,ASS,AT1,AV1,    C-01
     1        AV2,AW1,AW2,AZD,AZZ,A2D,A3D,A6D,                           C-02
     2        BB1,BB2,BB3,BB4,BB5,BB6,BB7,BB8,BB9,B10,B11,B12,BM,BP,     C-03
     3        CC,CN,CS,                                                  C-04
     4        DA1,DA2,DD,DDS,DR1,DR2,DT1,DV1,DV2,DW1,DW2,D12,            C-05
     5        ERR,FF,GG,HH,HS,                                           C-06
     6        II1,II2,II3,II4,ICC,INKODE,IRM,IRR,I3I,                    C-07
     7        KDCAL,KDGRD,KDPLT,KODE2,KODE6,KODE7,KODE8,K800,            C-08
     8        LL,LLM,LRM,                                                C-09
     9        NA1X,NA2X,NN1,NN2,NN3,NN4,NN5,NN6,NN7,NN8,NNN,NR1X,NR2X    C-10
      COMMON NTN,NTT,NT1,NV1X,NV2X,NW1X,NW2X,N3N,PL,                     C-11
     1        QQ,RR,SN,SS,TT,VC,VV,WW,WX,XC,XN,XX                        C-12
      DIMENSION BM(51),BP(51),                                           D-01
     1           CC(2,100),CN(90),CS(51),                                D-02
     2           DD(2,100),FF(2,51),GG(2,51),HH(90),HS(90),PL(51),       D-03
     3           QQ(50),RR(500),SS(500),SN(51),TT(500),VC(500),VV(500),  D-04
     4           WW(500),WX(90),                                         D-05
     5           XC(90),XN(90),XX(90)                                    D-06
      IF(K800) 899,898,899                                              8-002
  898 K800=1                                                            8-003
      ASSIGN 800 TO II1                                                 8-004
  899 GO TO II1, (800,811,812,813,814,815,816,817,818)                  8-005
C     SET ENTRY CHANNEL AND EXIT CHANNEL                                8-006
  800 Z=ERR                                                             8-007
      ASSIGN 890 TO II3                                                 8-008
      IF(DV1) 801,842,801                                               8-009
  801 ASSIGN 811 TO II1                                                 8-010
      ASSIGN 821 TO II2                                                 8-011
      J=0                                                               8-012
      GO TO 811                                                         8-013
  842 IF(DW1) 802,843,802                                               8-014
  802 ASSIGN 812 TO II1                                                 8-015
      ASSIGN 822 TO II2                                                 8-016
      J=0                                                               8-017
      GO TO 812                                                         8-018
  843 IF(DR1) 803,844,803                                               8-019
  803 ASSIGN 813 TO II1                                                 8-020
      ASSIGN 823 TO II2                                                 8-021
      J=0                                                               8-022
      GO TO 813                                                         8-023
  844 IF(DA1) 804,845,804                                               8-024
  804 ASSIGN 814 TO II1                                                 8-025
      ASSIGN 824 TO II2                                                 8-026
      J=0                                                               8-027
      GO TO 814                                                         8-028
  845 IF(DV2) 805,846,805                                               8-029
  805 ASSIGN 815 TO II1                                                 8-030
      ASSIGN 825 TO II2                                                 8-031
      J=0                                                               8-032
      GO TO 815                                                         8-033
  846 IF(DW2) 806,847,806                                               8-034
  806 ASSIGN 816 TO II1                                                 8-035
      ASSIGN 826 TO II2                                                 8-036
      J=0                                                               8-037
      GO TO 816                                                         8-038
  847 IF(DR2) 807,848,807                                               8-039
  807 ASSIGN 817 TO II1                                                 8-040
      ASSIGN 827 TO II2                                                 8-041
      J=0                                                               8-042
```

```
      GO TO 817
  848 IF(DA2) 808,849,808
  808 ASSIGN 818 TO II1
      ASSIGN 828 TO II2
      J=0
      GO TO 818
C     ENTRY CHANNELS
  811 E=AV1
      F=DV1
      GO TO II3,(890,891,892)
  812 E=AW1
      F=DW1
      GO TO II3,(890,891,892)
  813 E=AR1
      F=DR1
      GO TO II3,(890,891,892)
  814 E=AA1
      F=DA1
      GO TO II3,(890,891,892)
  815 E=AV2
      F=DV2
      GO TO II3,(890,891,892)
  816 E=AW2
      F=DW2
      GO TO II3,(890,891,892)
  817 E=AR2
      F=DR2
      GO TO II3,(890,891,892)
  818 E=AA2
      F=DA2
      GO TO II3,(890,891,892)
C     EXIT CHANNELS
  821 AV1=E
      IF(J) 895,895,842
  895 CONTINUE
      KODE8=2
      RETURN
  822 AW1=E
      IF(J) 895,895,843
  823 AR1=E
      IF(J) 894,894,844
  894 CONTINUE
      KODE8=1
      RETURN
  824 AA1=E
      IF(J) 894,894,845
  825 AV2=E
      IF(J) 895,895,846
  826 AW2=E
      IF(J) 895,895,847
  827 AR2=E
      IF(J) 894,894,848
  828 AA2=E
      IF(J) 894,894,849
C     FIRST STEP IN SEARCH
  890 ASSIGN 891 TO II3
      D = F
      X = ERR
      A = E
      E=E+D
      GO TO II2,(821,822,823,824,825,826,827,828)
```

```
C      SECOND STEP IN SEARCH
  891 ASSIGN 892 TO II3
      IF(X-ERR) 871,871,872
  871 Y=ERR
      B = E
      D = -D
      E = A+D
      GO TO II2,(821,822,823,824,825,826,827,828)
  872 Y = X
      B = A
      X = ERR
      A = E
      E = A+D
      GO TO II2,(821,822,823,824,825,826,827,828)
C      THIRD AND SUBSEQUENT STEPS IN SEARCH
  892 IF (X-ERR) 873,873,874
C      KEEP GOING IN SAME DIRECTION
  874 Y=X
      B=A
      X=ERR
      A=E
      E=A+D
      GO TO II2,(821,822,823,824,825,826,827,828)
C      GET BEST ESTIMATE OF E AND ERR AND GO ON TO NEXT VARIABLE
  873 G=(Y+ERR)/X-2.0
      IF(G-1.0E-6) 896,896,875
  875 G=0.5*(Y-ERR)/(X*G)
      E=A+D*G
      IF(G) 876,876,877
  876 ERR=X-(ERR-X)*G*G/(1.0-G-G)
      GO TO 896
  877 ERR=X-(Y-X)*G*G/(1.0+G+G)
  896 ASSIGN 890 TO II3
      J=1
      WRITE OUTPUT TAPE 6,888,ERR,E
  888 FORMAT(1H+27X,24HINTERPOLATIONS,   ERROR=1PE15.8,13H,  PARAMETER=
     11PE15.8)
      GO TO II2, (821,822,823,824,825,826,827,828)
C      END OF A CIRCUIT
  849 IF(ABSF(X-Z)/X-B10) 881,880,880
  880 NN7=NN7-1
      IF(NN7) 881,881,879
  879 II4=II4-1
      IF (II4) 882,882,800
  882 II4=NN6
      DV1=DV1*BB9
      DW1=DW1*BB9
      DR1=DR1*BB9
      DA1=DA1*BB9
      DV2=DV2*BB9
      DR2=DR2*BB9
      DA2=DA2*BB9
      DW2=DW2*BB9
      GO TO 800
  881 NN5=0
      KODE8=1
      RETURN
      END
```

APPENDIX B

SAMPLE DATA SET

Sample Input Data Listing

```
  TEST CASE,  CU-ALPHA,  39.8 MEV,  SEARCH ON R2, A2
   20    4    1   10    1    1    1   10   40   35    1    1    0    1
    1    1    1    1    1    1    1    1
48.       0.        6.82      .5        0.        0.        0.        0.
0.        14.       6.        .7        0.        0.        .1        -.02
39.8      6.8       .1        9.        4.        2.        63.       29.
20.       2.
     5.0+0     2.+0      1.+0      0.+0      1.-7      1.-8      1.-12     5.-4
      .5+0     1.-2      1.+0
24.       400.      1.        27.       180.      1.
29.5      77.       1.        30.5      37.       1.
32.       53.       1.        35.5      63.       1.
37.5      40.       1.        39.5      15.       1.
41.5      4.        1.        43.       10.       1.
46.       12.       1.        48.       9.        1.
50.       3.1       1.        52.       1.        1.
54.       2.5       1.        56.       3.6       1.
58.       3.1       1.        60.       1.8       1.
61.5      .62       1.        63.5      .53       1.
66.       1.        1.        68.       1.1       1.
70.       .8        1.        72.       .45       1.
74.       .17       1.        76.       .18       1.
78.5      .28       1.        79.5      .22       1.
81.5      .17       1.        84.       .091      1.
86.       .08       1.        88.       .09       1.
90.       .1        1.        91.5      .095      1.
94.       .05       1.
5.        -30.      1.        6.        0.        1.
```

Sample Output Data Listing

```
ELASTIC SCATTERING

 TEST CASE,  CU-ALPHA,  39.8 MEV,  SEARCH ON R2, A2

INPUT TO PART ONE

   AV1 = 4.79999995E 01     AW1 = 0.                AR1 = 6.81999999E 00     AA1 = 5.00000000E-01
   DV1 = 0.                 DW1 = 0.                DR1 = 0.                 DA1 = 0.
   AV2 = 0.                 AW2 = 1.39999999E 01    AR2 = 6.00000000E 00     AA2 = 6.99999994E-01
   DV2 = 0.                 DW2 = 0.                DR2 = 0.99999999E-01     DA2 =-1.99999997E-02
   AEE = 3.97999993E 01     ARC = 6.79999995E 00    DEL = 0.99999999E-01     ARR = 9.00000000E 00
   AMP = 4.00000000E 00     AZP = 2.00000000E 00    AMT = 6.29999995E 01     AZT = 2.89999998E 01
   AT1 = 1.99999999E 01     DT1 = 2.00000000E 00    NT1 =              40    NTT =              35
   BB1 = 5.00000000E 00     BB2 = 2.00000000E 00    BB3 = 1.00000000E 00     BB4 = 0.
   BB5 = 9.99999988E-08     BB6 = 9.99999988E-09    BB7 = 9.99999976E-13     BB8 = 4.99999994E-04
   BB9 = 5.00000000E-01     B10 = 9.99999988E-03    B11 = 1.00000000E 00
   NN1 =              20    NN2 =               4   NN3 =               1    NN4 =              10
   NN5 =               1    NN6 =               1   NN7 =               1    NN8 =              10
 NKODE =               1  KDPLT =               1 KDGRD =               0  KDCAL =               1
```

CM ANGLE (DEG)	CROSS SECTION (MB)	ERROR WEIGHT FACTOR
24.000	4.00000000E 02	1.00000000E 00
27.000	1.80000000E 02	1.00000000E 00
29.500	7.69999993E 01	1.00000000E 00
30.500	3.69999996E 01	1.00000000E 00
32.000	5.29999995E 01	1.00000000E 00
35.500	6.29999995E 01	1.00000000E 00
37.500	3.99999997E 01	1.00000000E 00
39.500	1.49999999E 01	1.00000000E 00
41.500	4.00000000E 00	1.00000000E 00
43.000	0.99999999E 01	1.00000000E 00
46.000	1.19999999E 01	1.00000000E 00
48.000	9.00000000E 00	1.00000000E 00
50.000	3.09999999E 00	1.00000000E 00
52.000	1.00000000E 00	1.00000000E 00
54.000	2.50000000E 00	1.00000000E 00
56.000	3.59999999E 00	1.00000000E 00
58.000	3.09999999E 00	1.00000000E 00
60.000	1.80000000E 00	1.00000000E 00
61.500	6.19999993E-01	1.00000000E 00
63.500	5.29999989E-01	1.00000000E 00
66.000	1.00000000E 00	1.00000000E 00
68.000	1.09999999E 00	1.00000000E 00
70.000	7.99999994E-01	1.00000000E 00
72.000	4.49999994E-01	1.00000000E 00
74.000	1.69999999E-01	1.00000000E 00
76.000	1.80000000E-01	1.00000000E 00
78.500	2.79999995E-01	1.00000000E 00
79.500	2.19999999E-01	1.00000000E 00
81.500	1.69999999E-01	1.00000000E 00
84.000	9.09999990E-02	1.00000000E 00
86.000	7.99999988E-02	1.00000000E 00
88.000	8.99999988E-02	1.00000000E 00
90.000	0.99999999E-01	1.00000000E 00
91.500	9.49999988E-02	1.00000000E 00
94.000	4.99999994E-02	1.00000000E 00

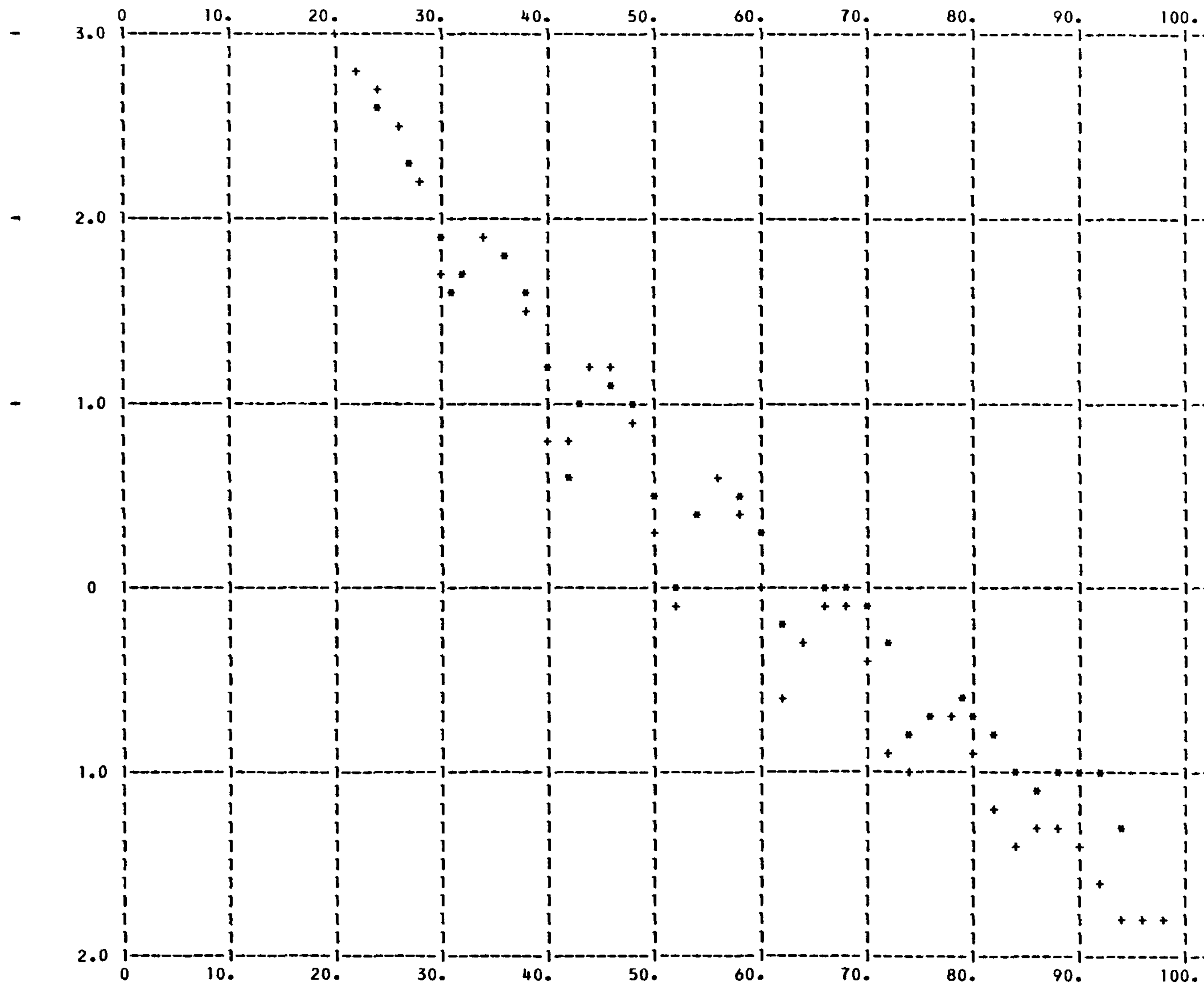
```
OUTPUT FROM PROGRAM

   AKK = 2.59434906E 00    ADD = 3.89999992E-02    AZZ = 2.89627042E 00    ACC = 4.76877314E-04

   ARR = 9.00899982E 00    ARM = 1.15829995E 01    IRR =            231    IRM =            264

   LRM =             30

RECURRENCE RELATIONS FOR COULOMB WAVE FUNCTION HAVE FAILED, INCREASE RMAX

   FINAL VALUE     ARM = 1.25189994E 01     IRM = 276

   FINAL VALUE     ARC = 6.78599989E 00     IRC = 174


   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 6.00000000E 00    AA2 = 6.99999994E-01
 ERROR = 5.80463213E 00

   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 6.09999996E 00    AA2 = 6.99999994E-01
 ERROR = 6.73265034E 00

   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 5.89999998E 00    AA2 = 6.99999994E-01
 ERROR = 5.47076815E 00

   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 5.79999995E 00    AA2 = 6.99999994E-01
 ERROR = 5.55709577E 00    INTERPOLATIONS,    ERROR= 5.45254004E 00,   PARAMETER= 5.87054473E 00

   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 5.87054473E 00    AA2 = 6.79999989E-01
 ERROR = 5.08810759E 00

   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 5.87054473E 00    AA2 = 6.59999985E-01
 ERROR = 5.02560300E 00

   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 5.87054473E 00    AA2 = 6.39999986E-01
 ERROR = 5.28400493E 00    INTERPOLATIONS,    ERROR= 5.01065475E 00,   PARAMETER= 6.66104484E-01

   MMM =                  0    LRM =                  30    LMAX =      28.000E 00
 FINAL PARAMETER VALUES
   AV1 = 4.79999995E 01    AW1 = 0.                      AR1 = 6.81999999E 00    AA1 = 5.00000000E-01
   AV2 = 0.                AW2 = 1.39999999E 01    AR2 = 5.87054473E 00    AA2 = 6.66104484E-01
 ERROR = 5.01065475E 00
```

CALCULATED VALUES OF ELASTIC CROSS SECTIONS

CM ANGLE (DEG)	EL XSCTN (MB)	COUL XSCTN (MB)	EL/COUL
20.000	9.62958920E 02	3.42673385E 03	2.81013629E-01
22.000	5.70692205E 02	2.35053077E 03	2.42792907E-01
24.000	4.88153476E 02	1.66742258E 03	2.92759302E-01
26.000	3.47278482E 02	1.21677208E 03	2.85409638E-01
28.000	1.54765056E 02	9.09621513E 02	1.70142256E-01
30.000	5.00323659E 01	6.94346786E 02	7.20567405E-02
32.000	5.44254661E 01	5.39770323E 02	1.00830786E-01
34.000	8.18312800E 01	4.26402742E 02	1.91910774E-01
36.000	6.98226541E 01	3.41689688E 02	2.04345217E-01
38.000	3.14305583E 01	2.77327996E 02	1.13333519E-01
40.000	6.26571721E 00	2.27695602E 02	2.75179541E-02
42.000	6.38151097E 00	1.88905549E 02	3.37814897E-02
44.000	1.50700368E 01	1.58219402E 02	9.52477157E-02
46.000	1.59072275E 01	1.33674738E 02	1.18999504E-01
48.000	8.70288706E 00	1.13843484E 02	7.64460701E-02
50.000	2.10061249E 00	9.76716113E 01	2.15068883E-02
52.000	8.18222284E-01	8.43710697E 01	9.69790089E-03
54.000	2.62395263E 00	7.33456379E 01	3.57751691E-02
56.000	3.55630508E 00	6.41393006E 01	5.54465818E-02
58.000	2.49202803E 00	5.63996542E 01	4.41851646E-02
60.000	9.05211937E-01	4.98518568E 01	1.81580383E-02
62.000	2.32998583E-01	4.42796361E 01	5.26198047E-03
64.000	4.70808333E-01	3.95114103E 01	1.19157560E-02
66.000	7.95787382E-01	3.54100302E 01	2.24735016E-02
68.000	7.09919691E-01	3.18650621E 01	2.22789359E-02
70.000	3.67436954E-01	2.87869832E 01	1.27639964E-02
72.000	1.28562714E-01	2.61027709E 01	4.92525154E-03
74.000	1.12168066E-01	2.37524977E 01	4.72236919E-03
76.000	1.82845095E-01	2.16866997E 01	8.43120873E-03
78.000	1.93067770E-01	1.98643412E 01	9.71931386E-03
80.000	1.29695812E-01	1.82511987E 01	7.10615301E-03
82.000	6.34438616E-02	1.68185945E 01	3.77224508E-03
84.000	3.98642811E-02	1.55423896E 01	2.56487462E-03
86.000	4.57365376E-02	1.44021747E 01	3.17566884E-03
88.000	4.89706349E-02	1.33806215E 01	3.65981761E-03
90.000	3.83481470E-02	1.24629647E 01	3.07696822E-03
92.000	2.40016937E-02	1.16365713E 01	2.06260872E-03
94.000	1.66017307E-02	1.08905929E 01	1.52441016E-03
96.000	1.58055563E-02	1.02156860E 01	1.54718500E-03
98.000	1.52522676E-02	9.60377419E 00	1.58815350E-03

Sample Output Data Plot

PLOT OF ELASTIC CROSS SECTION VS CM ANGLE (DEG)   NOTE - EXPERIMENTAL AND CALCULATED ANGLES ARE NOT THE SAME



* EXPERIMENTAL   + CALCULATED

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